



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2022 – 06:10 PM EST

PDB ID : 7JXT
Title : Ovine COX-1 in complex with the subtype-selective derivative 2a
Authors : Ko, Y.; Iaselli, M.; Miciaccia, M.; Friedrich, L.; Schneider, G.; Scilimati, A.; Cingolani, G.
Deposited on : 2020-08-27
Resolution : 3.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

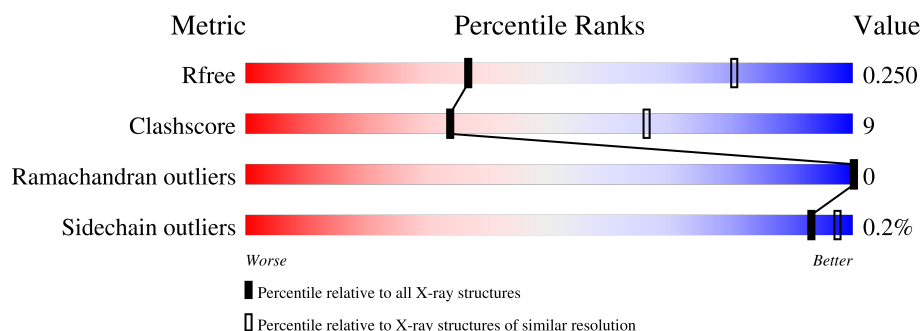
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 Å.

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



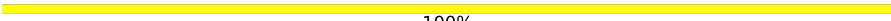
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	553	80% 20%
1	B	553	81% 18%
2	E	2	100%
2	F	2	50% 50%
2	G	2	100%
2	H	2	50% 50%
2	I	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	J	2	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18161 atoms, of which 8892 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	H	N	O	S	0	0	0
			8822	2900	4345	757	792	28			
1	B	553	Total	C	H	N	O	S	0	0	0
			8819	2900	4349	750	792	28			

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



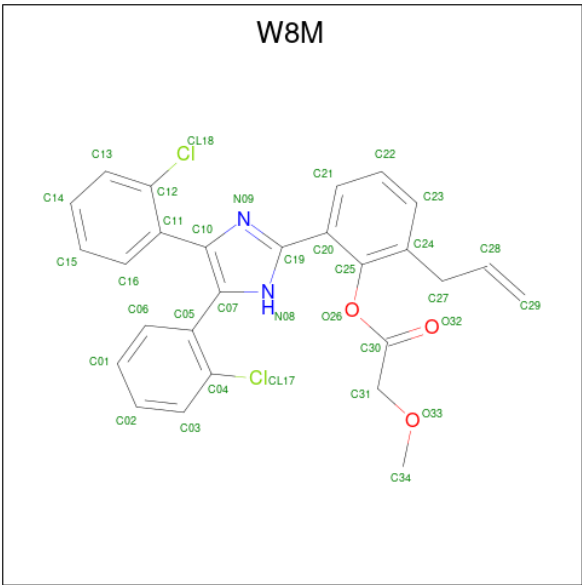
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	2	Total	C	H	N	O	0	0	0
			44	16	16	2	10			
2	F	2	Total	C	H	N	O	0	0	0
			44	16	16	2	10			
2	G	2	Total	C	H	N	O	0	0	0
			44	16	16	2	10			
2	H	2	Total	C	H	N	O	0	0	0
			44	16	16	2	10			
2	I	2	Total	C	H	N	O	0	0	0
			44	16	16	2	10			
2	J	2	Total	C	H	N	O	0	0	0
			44	16	16	2	10			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	B	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 4 is 2-[4,5-bis(2-chlorophenyl)-1H-imidazol-2-yl]-6-(prop-2-en-1-yl)phenyl methoxyacetate (three-letter code: W8M) (formula: C₂₇H₂₂Cl₂N₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	H	N	O	0	0
			55	27	2	21	2	3		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	Cl	H	N	O	0	0
			55	27	2	21	2	3		

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

Chain F:  50% 50%

MAG1
MAG2

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

Chain G:  100%

MAG1
MAG2

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

Chain H:  50% 50%

MAG1
MAG2

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

Chain I:  50% 50%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	181.60Å 181.60Å 103.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.99 – 3.35 14.99 – 3.35	Depositor EDS
% Data completeness (in resolution range)	83.2 (14.99-3.35) 83.1 (14.99-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.18	Depositor
R, R_{free}	0.210 , 0.250 0.212 , 0.250	Depositor DCC
R_{free} test set	1163 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	122.3	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.329 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18161	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, W8M, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/4616	0.45	0/6270
1	B	0.26	0/4609	0.44	0/6261
All	All	0.26	0/9225	0.44	0/12531

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4477	4345	4349	82	0
1	B	4470	4349	4347	70	0
2	E	28	16	25	0	0
2	F	28	16	25	1	0
2	G	28	16	25	0	0
2	H	28	16	25	1	0
2	I	28	16	25	1	0
2	J	28	16	25	0	0
3	A	43	30	30	5	0
3	B	43	30	30	6	0
4	A	34	21	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	34	21	0	2	0
All	All	9269	8892	8906	155	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 9.

All (155) 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:120:ARG:HD3	1:A:527:ALA:HB1	1.44	0.99
1:A:206:THR:HG21	1:A:385:TYR:CZ	2.03	0.94
1:A:161:THR:OG1	1:A:164:ASP:O	1.98	0.82
3:B:601:HEM:HBC2	3:B:601:HEM:HHD	1.62	0.81
3:A:601:HEM:HHD	3:A:601:HEM:HBC2	1.64	0.80
1:B:161:THR:OG1	1:B:164:ASP:O	1.97	0.80
1:A:104:ASN:O	1:A:109:ARG:NH1	2.17	0.78
1:A:238:LEU:HD12	2:I:1:NAG:H2	1.66	0.77
1:B:117:LEU:HD23	1:B:366:LEU:HG	1.65	0.76
1:B:238:LEU:HD12	2:F:1:NAG:H2	1.69	0.75
1:A:394:SER:OG	1:A:396:ARG:NH1	2.22	0.73
1:A:112:LEU:O	1:A:116:VAL:HG22	1.91	0.71
1:B:39:TYR:OH	1:B:163:MET:O	2.09	0.71
1:A:39:TYR:OH	1:A:163:MET:O	2.09	0.70
1:B:109:ARG:NH2	1:B:358:GLN:OE1	2.26	0.68
1:B:246:LEU:HD12	1:B:253:LYS:HA	1.77	0.66
1:B:117:LEU:HD11	4:B:602:W8M:C29	2.27	0.65
1:B:388:HIS:HB3	1:B:444:ILE:HD12	1.79	0.63
1:B:117:LEU:HB3	1:B:366:LEU:HD21	1.80	0.63
1:B:184:ARG:NH2	1:B:391:MET:O	2.30	0.62
1:A:184:ARG:NH2	1:A:391:MET:O	2.33	0.62
1:A:120:ARG:HD3	1:A:527:ALA:CB	2.24	0.62
3:A:601:HEM:HBB2	3:A:601:HEM:HMB2	1.82	0.62
3:B:601:HEM:HBB2	3:B:601:HEM:HMB2	1.82	0.62
1:A:568:VAL:HG21	1:A:578:VAL:HG21	1.82	0.61
1:A:388:HIS:HB3	1:A:444:ILE:HD12	1.83	0.61
1:A:206:THR:HG21	1:A:385:TYR:CE2	2.35	0.60
1:B:447:VAL:HG13	3:B:601:HEM:HBA1	1.82	0.60
1:A:491:LEU:HD11	1:A:509:LEU:HD13	1.84	0.60
1:A:120:ARG:CD	1:A:527:ALA:HB1	2.27	0.60
1:A:182:LEU:HB3	1:A:440:ILE:HD12	1.83	0.59
1:B:211:LYS:HD3	1:B:223:ALA:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ARG:NH2	1:B:459:ARG:O	2.36	0.59
1:A:179:ARG:HD3	1:A:183:LEU:HD22	1.86	0.56
1:B:568:VAL:HG21	1:B:578:VAL:HG21	1.87	0.56
1:A:366:LEU:HD13	1:A:371:PHE:CD2	2.40	0.56
1:A:211:LYS:HD3	1:A:223:ALA:HB2	1.87	0.56
1:B:517:ILE:HG23	1:B:518:PHE:CD2	2.41	0.56
1:A:287:VAL:HG21	1:A:292:PHE:HB2	1.88	0.55
1:A:517:ILE:HG23	1:A:518:PHE:CD2	2.42	0.55
1:B:172:PRO:O	1:B:456:ARG:NH2	2.40	0.54
1:A:340:THR:O	1:A:344:VAL:HG23	2.08	0.54
1:B:467:ARG:NH1	1:B:521:SER:OG	2.41	0.54
1:A:396:ARG:NH1	1:A:401:ASP:OD1	2.40	0.54
1:B:491:LEU:HD11	1:B:509:LEU:HD13	1.89	0.53
1:A:97:ARG:HG2	1:A:101:ASP:OD2	2.09	0.53
1:B:260:GLU:OE1	1:B:307:ARG:NH1	2.41	0.53
1:A:385:TYR:HD1	1:A:385:TYR:O	1.91	0.53
1:A:545:TRP:O	1:B:61:ARG:NH2	2.32	0.53
1:B:113:MET:HB3	1:B:365:LEU:HD13	1.89	0.53
1:B:423:VAL:HG11	1:B:568:VAL:HG11	1.91	0.53
1:A:572:THR:OG1	1:A:574:THR:O	2.18	0.53
1:A:61:ARG:NH2	1:B:545:TRP:O	2.34	0.52
1:B:484:GLU:OE2	1:B:487:MET:HB3	2.09	0.52
1:A:447:VAL:O	1:A:451:VAL:HG23	2.10	0.52
1:B:323:TRP:HE3	1:B:328:LEU:HD23	1.74	0.52
1:A:230:LEU:HD22	1:A:233:ILE:HD12	1.92	0.52
1:A:246:LEU:HD12	1:A:253:LYS:HA	1.92	0.52
1:A:206:THR:CG2	1:A:385:TYR:CZ	2.87	0.52
1:A:196:LEU:HD11	1:A:392:PRO:HG3	1.92	0.51
3:A:601:HEM:HBB2	3:A:601:HEM:CMB	2.41	0.50
1:B:113:MET:O	1:B:117:LEU:HD13	2.11	0.50
3:B:601:HEM:HBB2	3:B:601:HEM:CMB	2.41	0.50
1:B:340:THR:O	1:B:344:VAL:HG23	2.11	0.50
1:B:478:PHE:HE1	1:B:501:LEU:HD13	1.77	0.50
1:A:291:VAL:HG13	1:A:294:LEU:HD12	1.93	0.49
1:B:447:VAL:O	1:B:451:VAL:HG23	2.12	0.49
1:A:209:PHE:HB2	1:A:377:ILE:HG13	1.93	0.49
1:A:484:GLU:OE2	1:A:487:MET:HB3	2.12	0.49
1:A:467:ARG:NH1	1:A:521:SER:OG	2.46	0.49
1:B:83:ARG:NE	1:B:83:ARG:HA	2.28	0.48
1:B:543:GLU:O	1:B:546:LYS:NZ	2.46	0.48
1:A:232:HIS:CD2	1:A:233:ILE:HG13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:VAL:HA	1:B:348:TYR:HB3	1.96	0.48
1:B:232:HIS:CD2	1:B:233:ILE:HG13	2.49	0.48
1:B:172:PRO:HB3	1:B:494:LEU:HD23	1.95	0.48
1:A:172:PRO:O	1:A:456:ARG:NH2	2.45	0.48
1:A:344:VAL:HA	1:A:348:TYR:HB3	1.97	0.47
1:A:106:THR:HG23	1:A:108:ILE:H	1.80	0.47
1:A:478:PHE:HE1	1:A:501:LEU:HD13	1.80	0.47
1:B:121:SER:HB3	1:B:531:LEU:HD22	1.96	0.47
1:A:423:VAL:HG11	1:A:568:VAL:HG11	1.96	0.47
1:B:182:LEU:HB3	1:B:440:ILE:HD12	1.96	0.47
1:B:380:GLU:HG2	1:B:466:TYR:CE2	2.50	0.47
1:A:300:LEU:HD11	1:A:419:VAL:HG13	1.97	0.47
1:A:554:VAL:O	1:A:558:LEU:HD13	2.15	0.47
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.50	0.46
1:A:352:LEU:HD23	4:A:602:W8M:CL18	2.53	0.46
1:B:175:GLU:HG2	1:B:449:VAL:HG11	1.96	0.46
1:A:208:GLN:HB3	1:A:232:HIS:ND1	2.30	0.46
1:B:433:ARG:O	1:B:439:ASN:ND2	2.46	0.46
1:A:447:VAL:HG13	3:A:601:HEM:HBA1	1.98	0.46
1:B:196:LEU:HD11	1:B:392:PRO:HG3	1.97	0.46
1:B:230:LEU:HD22	1:B:233:ILE:HD12	1.97	0.46
1:A:121:SER:HB3	1:A:531:LEU:HD22	1.98	0.46
1:B:386:HIS:ND1	1:B:451:VAL:HG21	2.30	0.46
1:B:389:PRO:HB2	1:B:434:ILE:HA	1.97	0.46
1:B:554:VAL:O	1:B:558:LEU:HD13	2.16	0.46
1:B:391:MET:SD	3:B:601:HEM:HAB	2.56	0.45
1:A:260:GLU:OE1	1:A:307:ARG:NH1	2.50	0.45
1:A:386:HIS:ND1	1:A:451:VAL:HG21	2.31	0.45
1:A:113:MET:HB3	1:A:365:LEU:HD13	1.98	0.45
1:A:344:VAL:CG1	1:A:534:LEU:HD21	2.46	0.45
1:B:291:VAL:O	1:B:291:VAL:HG12	2.17	0.45
1:A:172:PRO:HB3	1:A:494:LEU:HD23	1.98	0.45
1:B:67:PRO:HG2	2:H:1:NAG:H82	1.98	0.44
1:A:115:LEU:C	1:A:115:LEU:HD23	2.37	0.44
1:A:567:LEU:O	1:A:571:ASN:ND2	2.48	0.44
1:B:93:LEU:HD13	1:B:355:TYR:CZ	2.52	0.44
1:B:206:THR:HG21	1:B:385:TYR:CE2	2.53	0.44
1:B:209:PHE:HB2	1:B:377:ILE:HG13	1.98	0.44
1:A:385:TYR:O	1:A:385:TYR:CD1	2.70	0.44
1:A:80:THR:O	1:A:83:ARG:HG2	2.18	0.44
1:A:113:MET:CE	4:A:602:W8M:C29	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ARG:O	1:B:83:ARG:HG2	2.17	0.43
1:B:344:VAL:HG11	1:B:534:LEU:HD21	2.00	0.43
1:A:530:SER:O	1:A:534:LEU:HD13	2.19	0.43
1:A:291:VAL:HG12	1:A:291:VAL:O	2.19	0.43
1:A:344:VAL:O	1:A:348:TYR:HB3	2.18	0.43
1:B:567:LEU:O	1:B:571:ASN:ND2	2.51	0.43
1:A:323:TRP:CE3	1:A:327:GLN:HG3	2.54	0.43
1:B:106:THR:HG23	1:B:108:ILE:H	1.84	0.43
1:B:208:GLN:HB3	1:B:232:HIS:ND1	2.33	0.43
1:A:234:TYR:O	1:A:241:GLN:HB3	2.19	0.42
1:B:64:TYR:CE1	1:B:76:THR:HG21	2.54	0.42
1:A:279:ILE:HD11	1:A:411:THR:HB	2.00	0.42
1:A:344:VAL:HG11	1:A:534:LEU:HD21	2.01	0.42
1:A:554:VAL:HG23	1:A:555:GLY:N	2.34	0.42
1:A:324:GLY:O	1:A:328:LEU:HD23	2.19	0.42
1:B:344:VAL:CG1	1:B:534:LEU:HD21	2.50	0.42
1:B:292:PHE:CD1	1:B:298:LEU:HD23	2.54	0.42
1:B:130:TYR:HB2	1:B:150:ARG:HB3	2.01	0.42
1:B:388:HIS:N	1:B:389:PRO:CD	2.82	0.42
1:B:554:VAL:HG23	1:B:555:GLY:N	2.34	0.42
1:A:198:PHE:CZ	1:A:352:LEU:HD13	2.55	0.42
1:A:113:MET:O	1:A:117:LEU:CB	2.68	0.41
1:B:120:ARG:NH2	4:B:602:W8M:C15	2.83	0.41
1:B:530:SER:O	1:B:534:LEU:HD13	2.20	0.41
1:A:389:PRO:HB2	1:A:434:ILE:HA	2.02	0.41
1:A:394:SER:HG	1:A:396:ARG:NH1	2.18	0.41
1:A:548:SER:HB3	1:B:58:ASP:HB2	2.03	0.41
1:B:246:LEU:CD2	1:B:248:LYS:HB3	2.50	0.41
1:B:287:VAL:HG21	1:B:292:PHE:HB2	2.02	0.41
1:A:150:ARG:NH2	1:A:459:ARG:O	2.47	0.41
1:A:197:MET:O	1:A:301:TYR:OH	2.30	0.41
1:A:205:PHE:O	1:A:208:GLN:HG2	2.21	0.41
1:A:109:ARG:O	1:A:113:MET:HG2	2.21	0.41
1:B:295:LEU:HD21	3:B:601:HEM:CBB	2.52	0.40
1:B:253:LYS:O	1:B:264:PRO:HD3	2.21	0.40
1:A:391:MET:SD	3:A:601:HEM:HAB	2.62	0.40
1:B:402:TYR:HH	1:B:417:TYR:HE2	1.69	0.40
1:A:206:THR:CG2	1:A:385:TYR:CE2	3.04	0.40
1:A:279:ILE:O	1:A:279:ILE:HG23	2.21	0.40
1:A:397:VAL:HA	1:A:425:ALA:HB1	2.02	0.40
1:B:345:ILE:HD12	1:B:361:PHE:CD1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	551/553 (100%)	531 (96%)	20 (4%)	0	100	100
1	B	551/553 (100%)	534 (97%)	17 (3%)	0	100	100
All	All	1102/1106 (100%)	1065 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	484/490 (99%)	483 (100%)	1 (0%)	93	97
1	B	484/490 (99%)	483 (100%)	1 (0%)	93	97
All	All	968/980 (99%)	966 (100%)	2 (0%)	93	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	385	TYR
1	B	385	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

12 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	2,1	14,14,15	1.36	2 (14%)	17,19,21	1.23	3 (17%)
2	NAG	E	2	2	14,14,15	1.34	1 (7%)	17,19,21	1.21	3 (17%)
2	NAG	F	1	2,1	14,14,15	1.38	2 (14%)	17,19,21	1.27	3 (17%)
2	NAG	F	2	2	14,14,15	1.34	1 (7%)	17,19,21	1.12	3 (17%)
2	NAG	G	1	2,1	14,14,15	1.41	3 (21%)	17,19,21	1.16	1 (5%)
2	NAG	G	2	2	14,14,15	1.37	1 (7%)	17,19,21	1.11	1 (5%)
2	NAG	H	1	2,1	14,14,15	1.33	1 (7%)	17,19,21	1.24	3 (17%)
2	NAG	H	2	2	14,14,15	1.35	2 (14%)	17,19,21	1.17	2 (11%)
2	NAG	I	1	2,1	14,14,15	1.42	2 (14%)	17,19,21	1.14	2 (11%)
2	NAG	I	2	2	14,14,15	1.33	1 (7%)	17,19,21	1.16	3 (17%)
2	NAG	J	1	2,1	14,14,15	1.40	3 (21%)	17,19,21	1.29	3 (17%)
2	NAG	J	2	2	14,14,15	1.36	1 (7%)	17,19,21	1.13	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	3/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	NAG	C7-N2	3.37	1.45	1.34
2	G	2	NAG	C7-N2	3.36	1.45	1.34
2	E	2	NAG	C7-N2	3.32	1.45	1.34
2	J	2	NAG	C7-N2	3.32	1.45	1.34
2	G	1	NAG	C7-N2	3.32	1.45	1.34
2	I	2	NAG	C7-N2	3.32	1.45	1.34
2	J	1	NAG	C7-N2	3.29	1.45	1.34
2	I	1	NAG	C7-N2	3.29	1.45	1.34
2	F	1	NAG	C7-N2	3.26	1.45	1.34
2	H	2	NAG	C7-N2	3.25	1.45	1.34
2	H	1	NAG	C7-N2	3.24	1.45	1.34
2	E	1	NAG	C7-N2	3.24	1.45	1.34
2	I	1	NAG	O5-C1	-2.40	1.39	1.43
2	G	1	NAG	O5-C1	-2.37	1.39	1.43
2	J	1	NAG	O5-C1	-2.33	1.40	1.43
2	F	1	NAG	O5-C1	-2.24	1.40	1.43
2	E	1	NAG	O5-C1	-2.06	1.40	1.43
2	H	2	NAG	O5-C1	-2.05	1.40	1.43
2	J	1	NAG	O7-C7	-2.02	1.18	1.23
2	G	1	NAG	O7-C7	-2.02	1.18	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C1-O5-C5	2.91	116.14	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	NAG	C1-C2-N2	-2.76	105.77	110.49
2	H	1	NAG	C2-N2-C7	-2.67	119.09	122.90
2	J	1	NAG	C8-C7-N2	2.59	120.49	116.10
2	G	1	NAG	C8-C7-N2	2.59	120.48	116.10
2	I	2	NAG	C4-C3-C2	-2.46	107.41	111.02
2	H	2	NAG	C8-C7-N2	2.41	120.18	116.10
2	H	1	NAG	C8-C7-N2	2.40	120.16	116.10
2	E	1	NAG	C2-N2-C7	-2.39	119.50	122.90
2	I	2	NAG	O5-C1-C2	-2.38	107.53	111.29
2	E	1	NAG	O5-C1-C2	-2.37	107.55	111.29
2	H	2	NAG	C2-N2-C7	-2.36	119.55	122.90
2	E	2	NAG	C8-C7-N2	2.33	120.04	116.10
2	J	2	NAG	C8-C7-N2	2.31	120.01	116.10
2	G	2	NAG	C8-C7-N2	2.29	119.97	116.10
2	E	1	NAG	C8-C7-N2	2.28	119.95	116.10
2	I	1	NAG	C8-C7-N2	2.25	119.90	116.10
2	F	2	NAG	C4-C3-C2	-2.23	107.75	111.02
2	I	1	NAG	C2-N2-C7	-2.20	119.77	122.90
2	F	1	NAG	C8-C7-N2	2.19	119.80	116.10
2	J	2	NAG	O5-C1-C2	-2.17	107.86	111.29
2	F	2	NAG	O5-C1-C2	-2.16	107.88	111.29
2	E	2	NAG	C6-C5-C4	-2.15	107.97	113.00
2	H	1	NAG	O5-C1-C2	-2.10	107.97	111.29
2	E	2	NAG	C2-N2-C7	-2.09	119.93	122.90
2	F	1	NAG	C2-N2-C7	-2.08	119.94	122.90
2	J	1	NAG	C2-N2-C7	-2.08	119.94	122.90
2	I	2	NAG	C8-C7-N2	2.06	119.59	116.10
2	J	2	NAG	C2-N2-C7	-2.06	119.98	122.90
2	F	2	NAG	C8-C7-N2	2.02	119.53	116.10

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6

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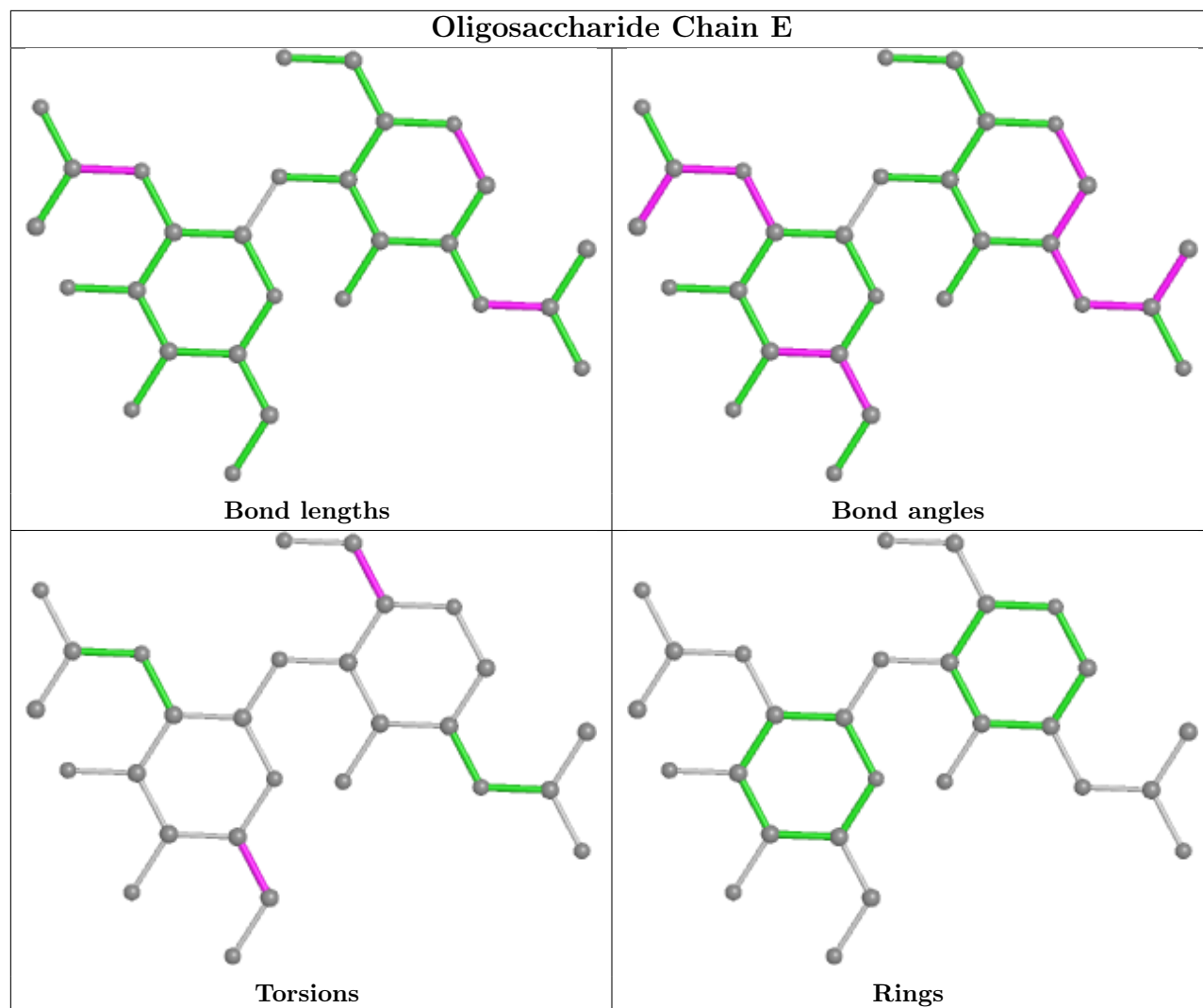
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C3-C2-N2-C7
2	I	2	NAG	C3-C2-N2-C7
2	E	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C1-C2-N2-C7

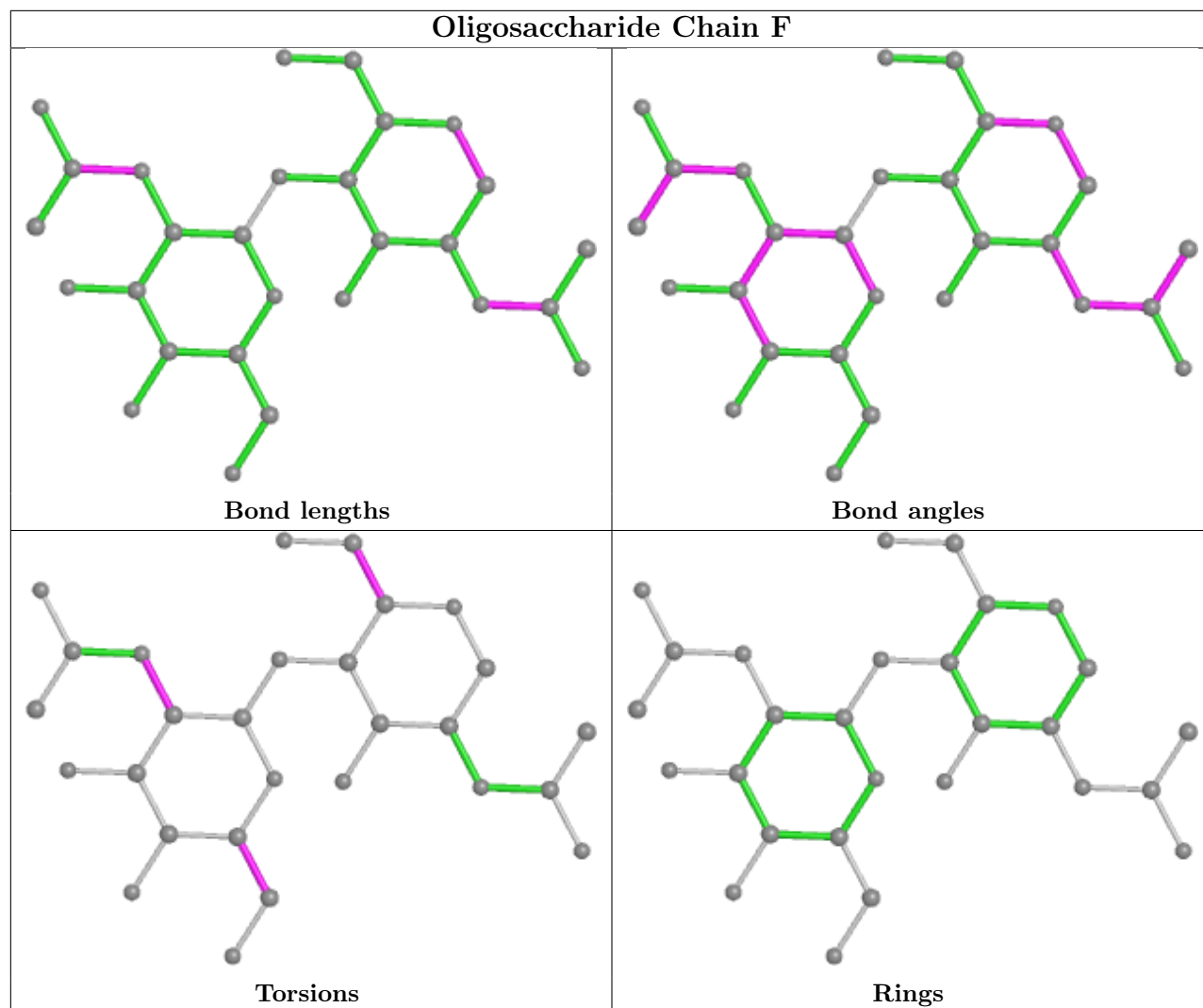
There are no ring outliers.

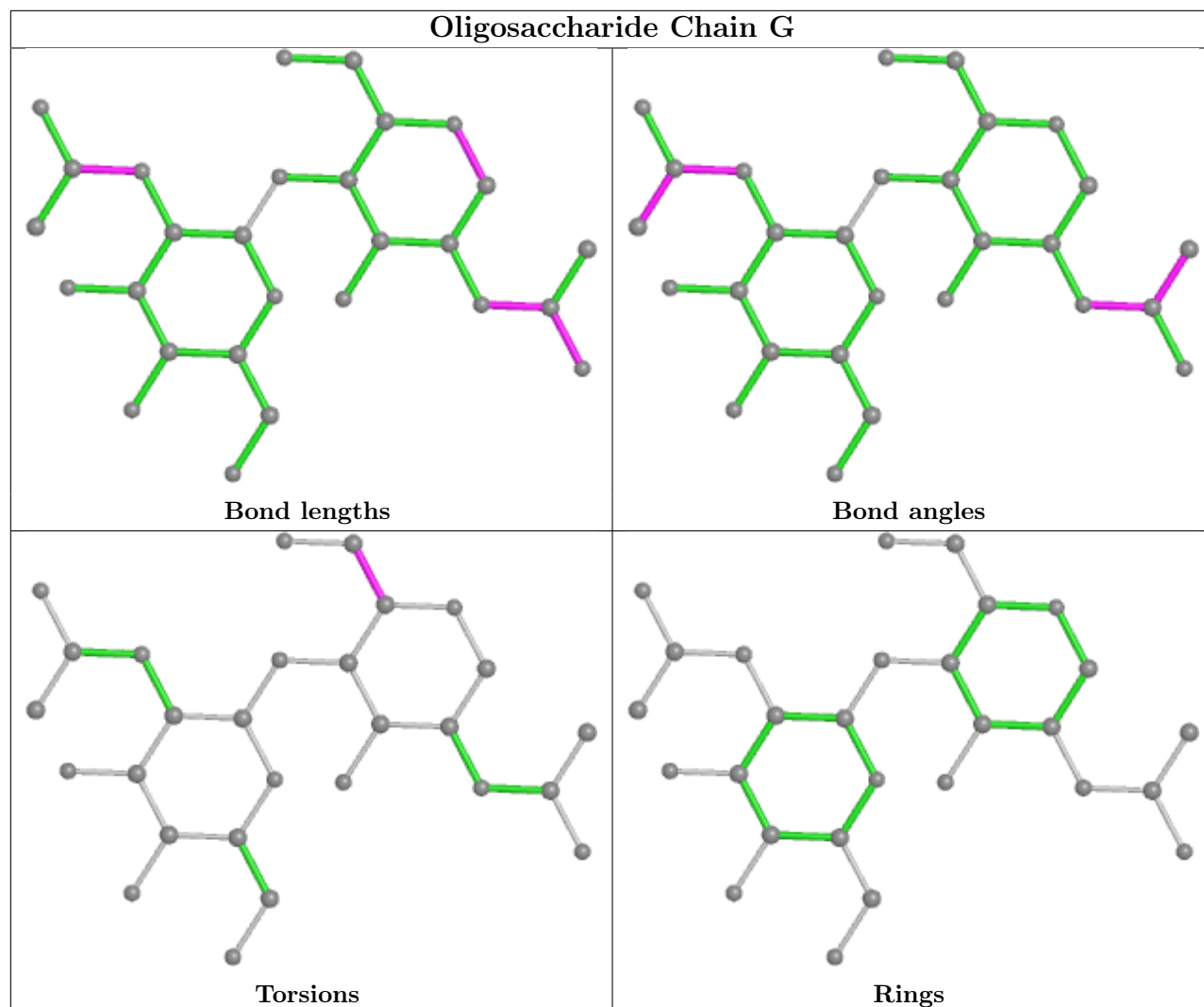
3 monomers are involved in 3 short contacts:

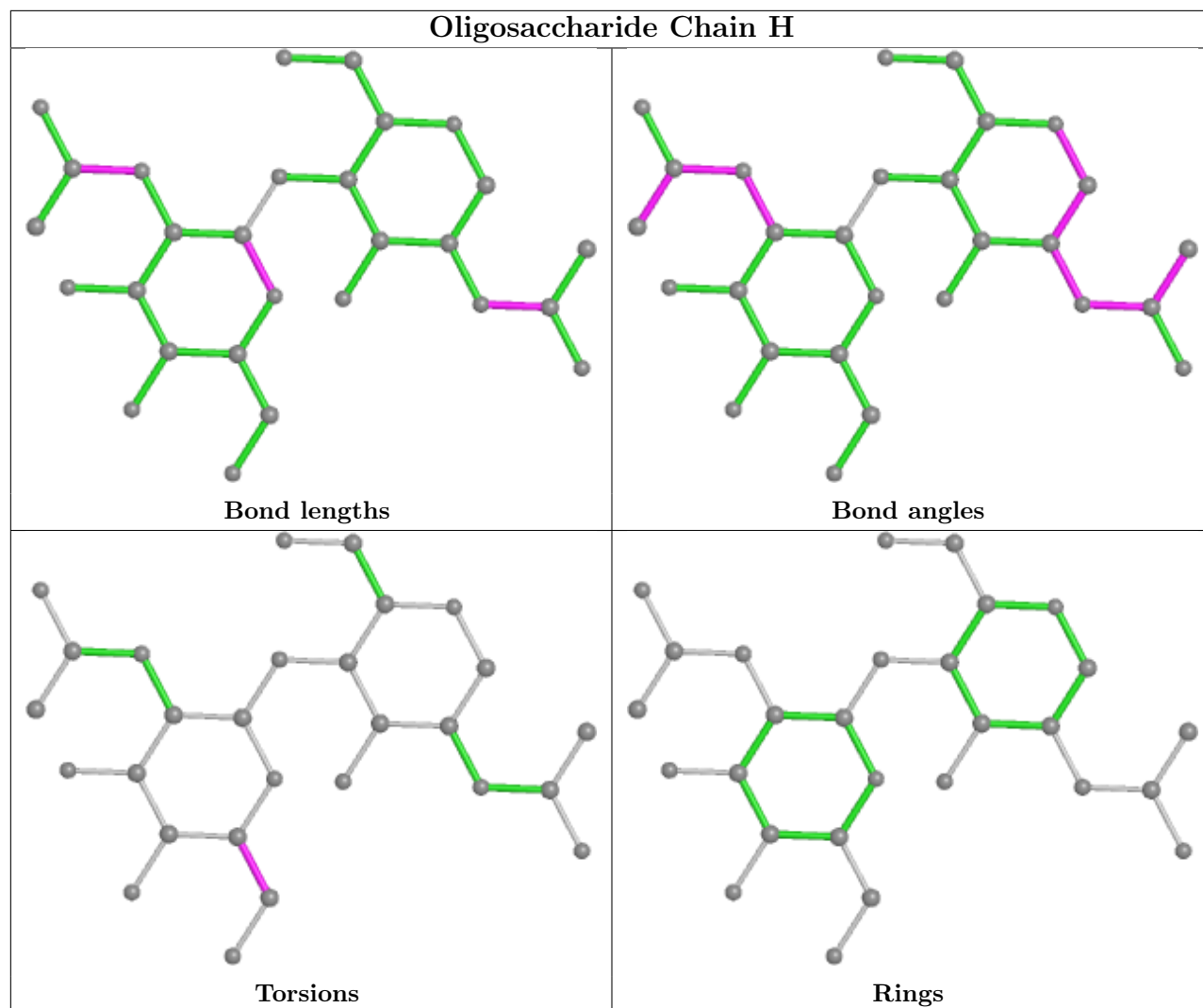
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1	NAG	1	0
2	H	1	NAG	1	0
2	F	1	NAG	1	0

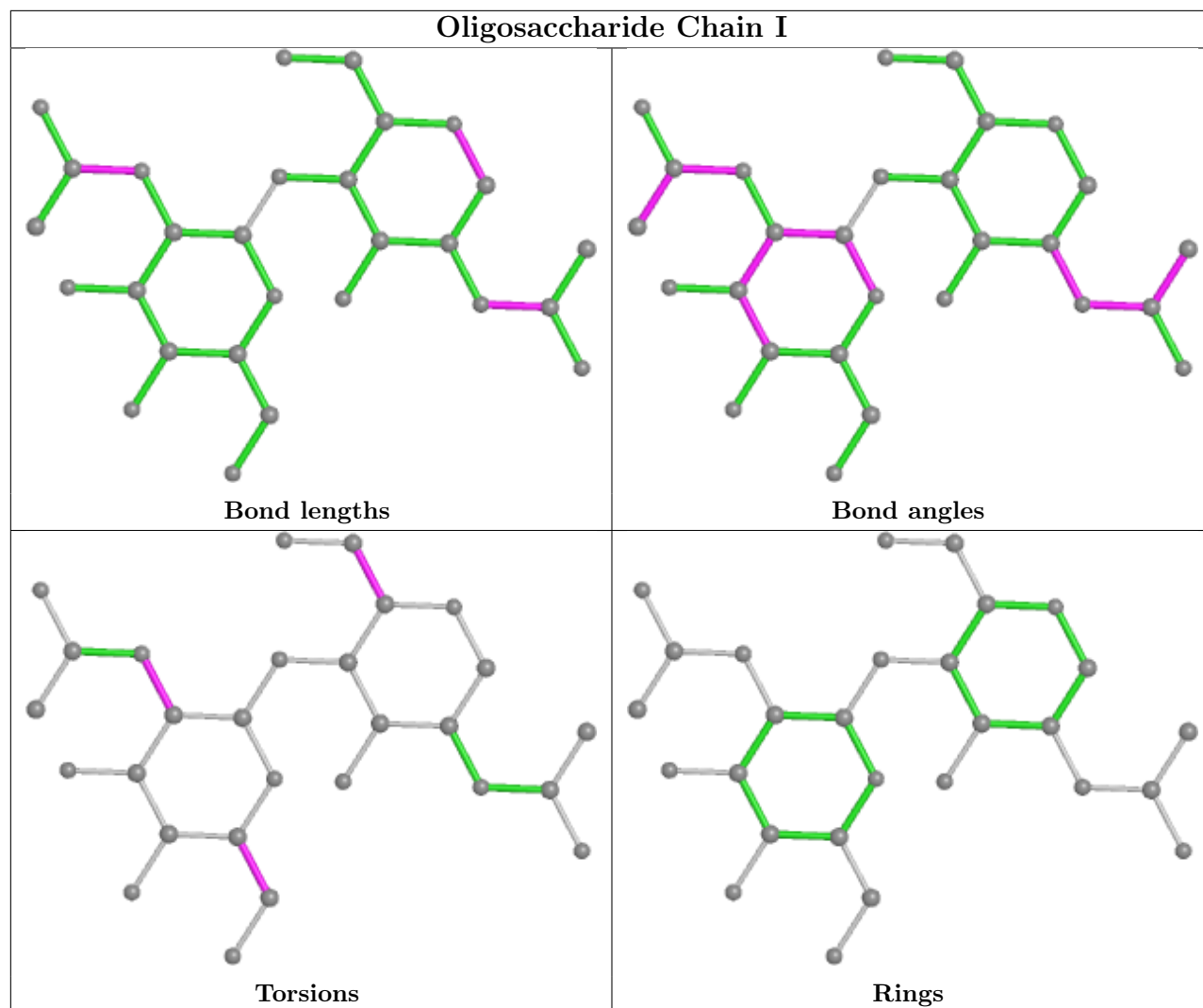
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

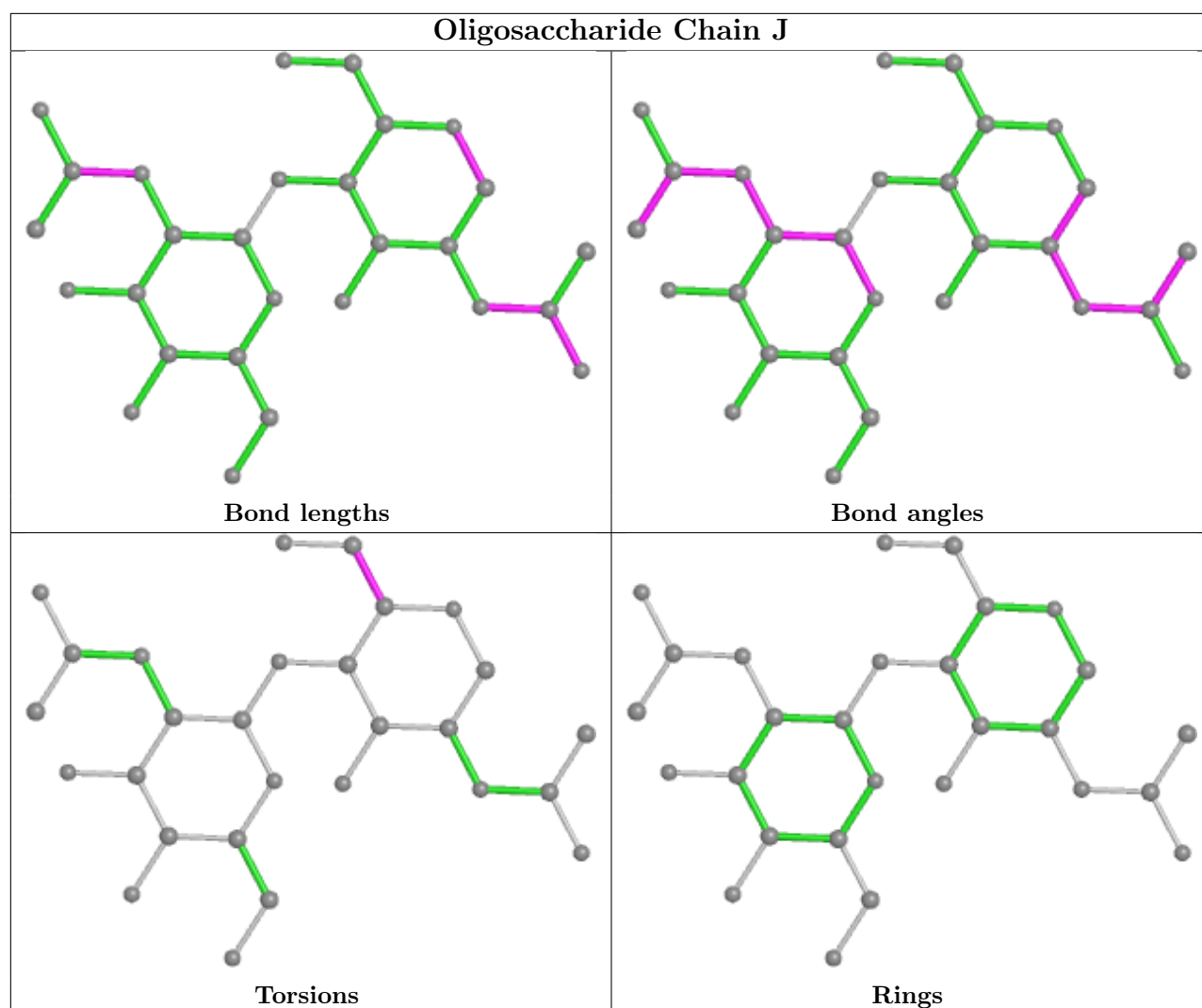












5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	A	601	-	27,50,50	1.90	5 (18%)	17,82,82	1.47	2 (11%)
4	W8M	A	602	-	37,37,37	1.44	6 (16%)	42,51,51	1.45	6 (14%)
3	HEM	B	601	1	27,50,50	1.89	5 (18%)	17,82,82	1.49	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	W8M	B	602	-	37,37,37	1.42	7 (18%)	42,51,51	1.41	5 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	601	-	-	2/6/54/54	-
4	W8M	A	602	-	-	6/20/22/22	0/4/4/4
3	HEM	B	601	1	-	2/6/54/54	-
4	W8M	B	602	-	-	6/20/22/22	0/4/4/4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	HEM	C3C-C2C	-4.39	1.34	1.40
3	B	601	HEM	C3C-C2C	-4.35	1.34	1.40
4	A	602	W8M	C05-C07	4.35	1.53	1.49
4	B	602	W8M	C05-C07	4.29	1.53	1.49
3	B	601	HEM	C3B-C2B	-4.14	1.34	1.40
3	A	601	HEM	C3B-C2B	-4.11	1.34	1.40
3	A	601	HEM	C3C-CAC	3.74	1.55	1.47
3	B	601	HEM	C3C-CAC	3.70	1.55	1.47
4	A	602	W8M	C11-C10	3.57	1.53	1.49
3	A	601	HEM	C3B-CAB	3.56	1.55	1.47
3	B	601	HEM	C3B-CAB	3.55	1.55	1.47
4	B	602	W8M	C11-C10	3.20	1.52	1.49
4	A	602	W8M	C07-C10	-2.74	1.37	1.44
4	B	602	W8M	C07-C10	-2.73	1.37	1.44
4	B	602	W8M	C10-N09	-2.73	1.30	1.37
4	A	602	W8M	C10-N09	-2.59	1.31	1.37
4	A	602	W8M	C04-CL17	2.26	1.79	1.73
4	B	602	W8M	C04-CL17	2.25	1.79	1.73
3	B	601	HEM	CAA-C2A	2.11	1.55	1.52
4	A	602	W8M	C12-CL18	2.08	1.78	1.73
3	A	601	HEM	CAA-C2A	2.08	1.55	1.52
4	B	602	W8M	C19-N09	-2.07	1.33	1.35
4	B	602	W8M	C12-CL18	2.06	1.78	1.73

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	W8M	C20-C19-N08	4.58	129.52	123.67
4	A	602	W8M	C20-C19-N08	4.30	129.16	123.67
4	A	602	W8M	C25-O26-C30	-4.15	110.81	116.96
4	B	602	W8M	C10-C11-C12	3.35	126.17	121.16
4	B	602	W8M	C16-C11-C10	-2.91	114.04	119.46
3	B	601	HEM	CMD-C2D-C1D	-2.57	124.51	128.46
4	B	602	W8M	C10-C07-N08	-2.55	106.89	113.76
3	A	601	HEM	CMD-C2D-C1D	-2.53	124.58	128.46
4	A	602	W8M	C10-C07-N08	-2.46	107.11	113.76
4	A	602	W8M	C10-C11-C12	2.46	124.83	121.16
3	B	601	HEM	CAD-CBD-CGD	-2.40	108.65	112.67
4	A	602	W8M	C07-C10-N09	-2.31	107.51	113.76
3	A	601	HEM	C1D-C2D-C3D	2.08	108.44	107.00
4	B	602	W8M	C07-C10-N09	-2.08	108.14	113.76
4	A	602	W8M	C16-C11-C10	-2.06	115.63	119.46

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	W8M	C07-C10-C11-C12
4	B	602	W8M	C07-C10-C11-C12
4	B	602	W8M	C04-C05-C07-C10
4	A	602	W8M	O32-C30-O26-C25
4	B	602	W8M	O32-C30-O26-C25
4	A	602	W8M	C31-C30-O26-C25
4	B	602	W8M	C31-C30-O26-C25
4	A	602	W8M	O32-C30-C31-O33
4	A	602	W8M	O26-C30-C31-O33
4	B	602	W8M	O32-C30-C31-O33
4	B	602	W8M	O26-C30-C31-O33
3	A	601	HEM	C2D-C3D-CAD-CBD
3	A	601	HEM	C4D-C3D-CAD-CBD
3	B	601	HEM	C2D-C3D-CAD-CBD
3	B	601	HEM	C4D-C3D-CAD-CBD
4	A	602	W8M	C04-C05-C07-C10

There are no ring outliers.

4 monomers are involved in 15 short contacts:

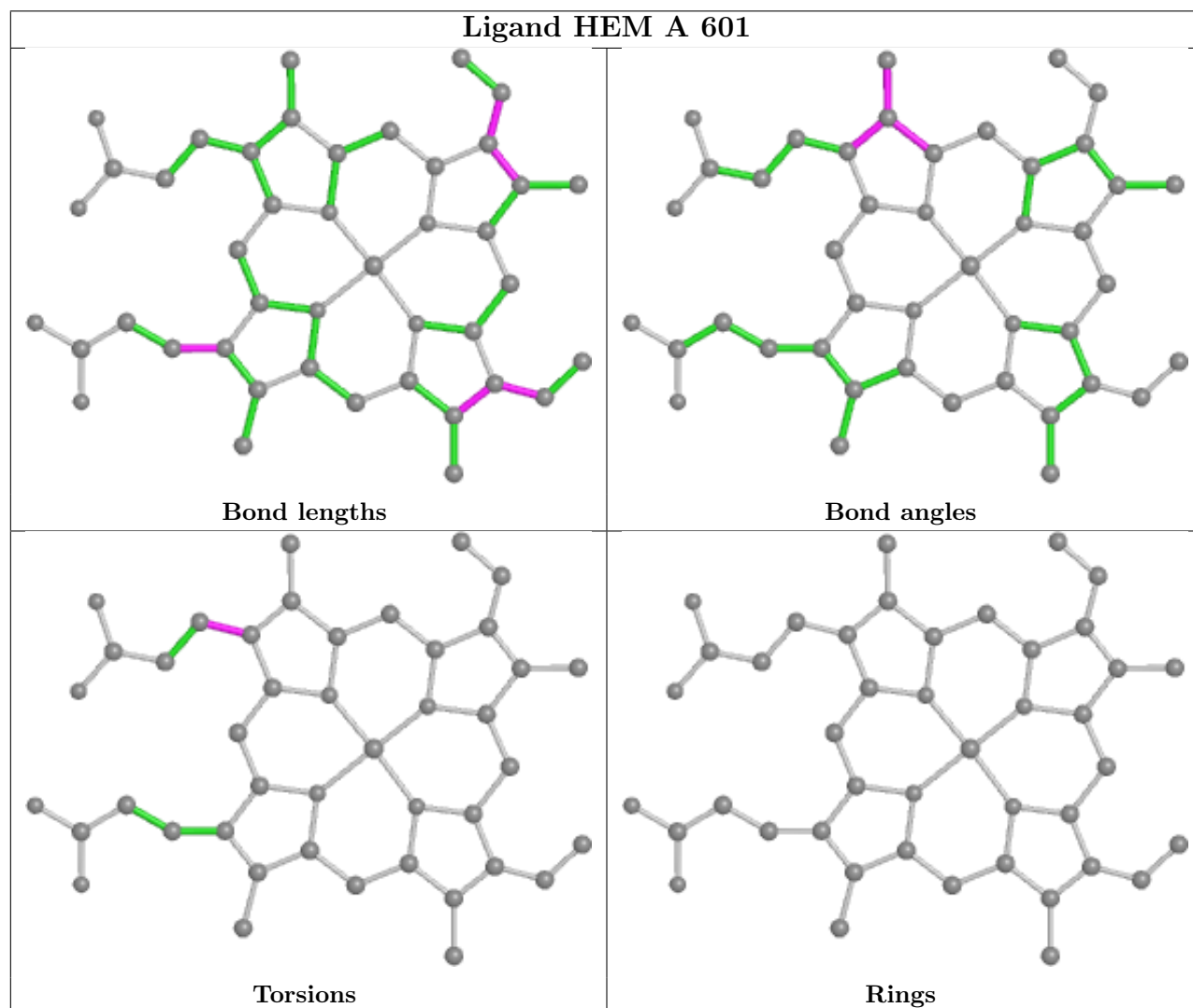
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	HEM	5	0

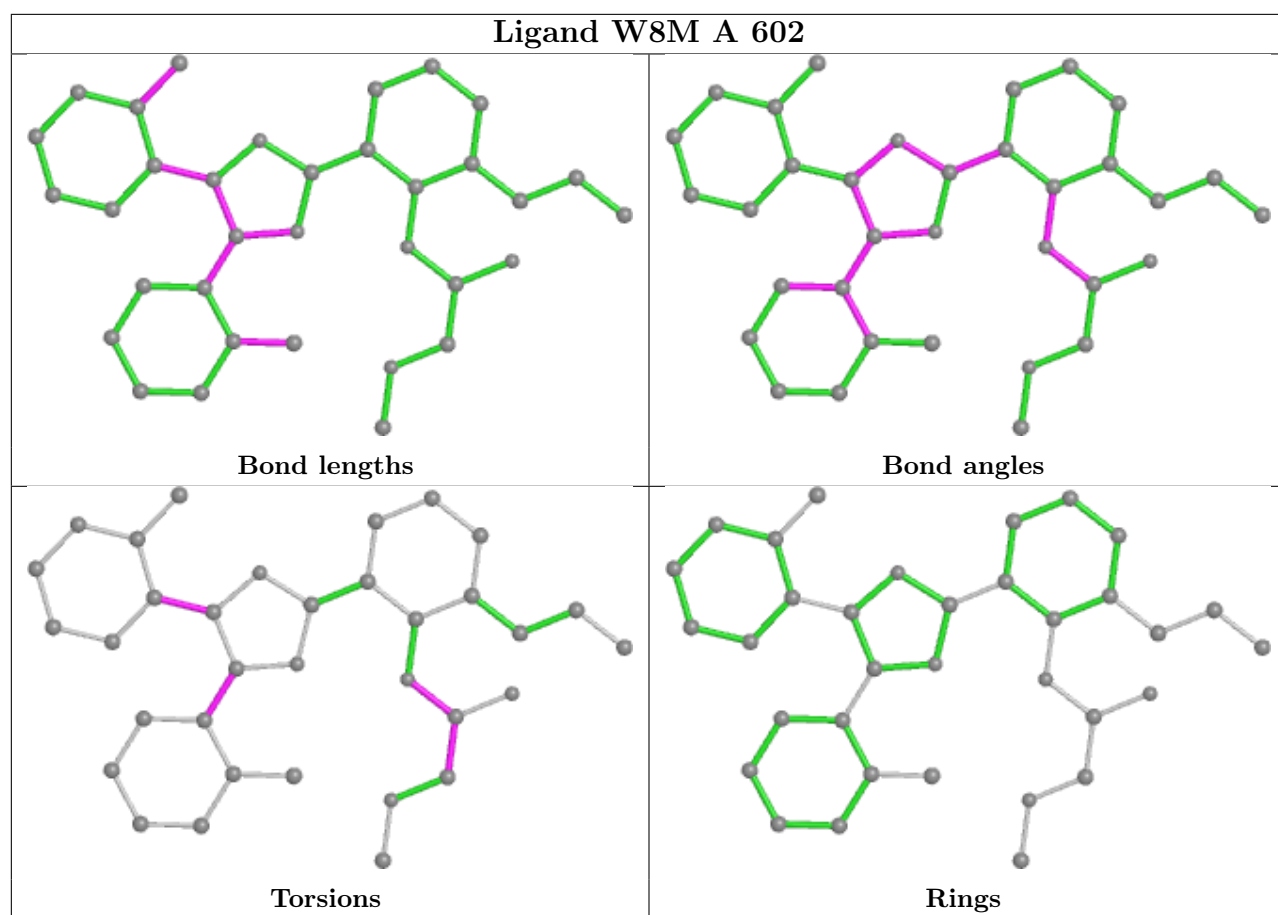
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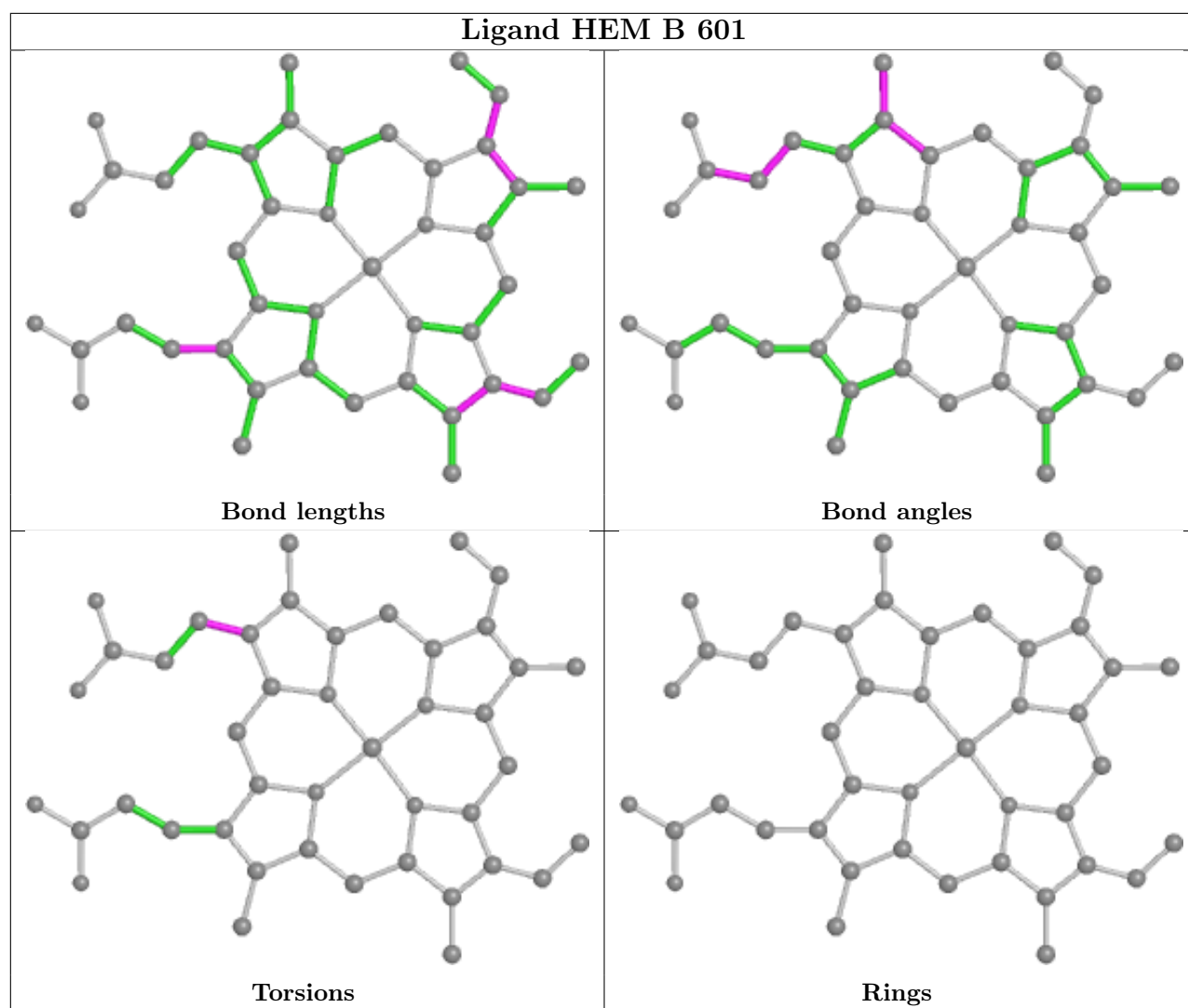
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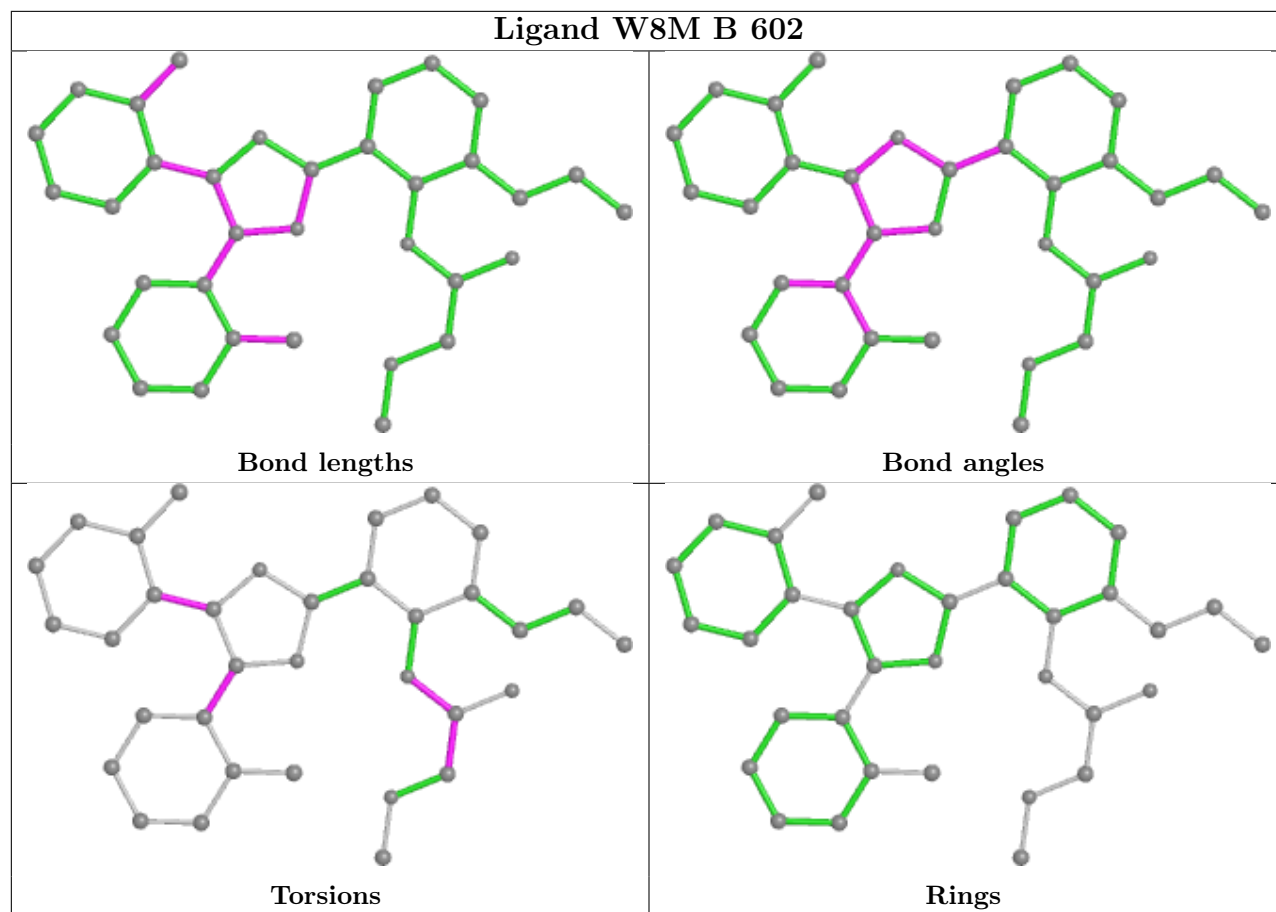
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	W8M	2	0
3	B	601	HEM	6	0
4	B	602	W8M	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

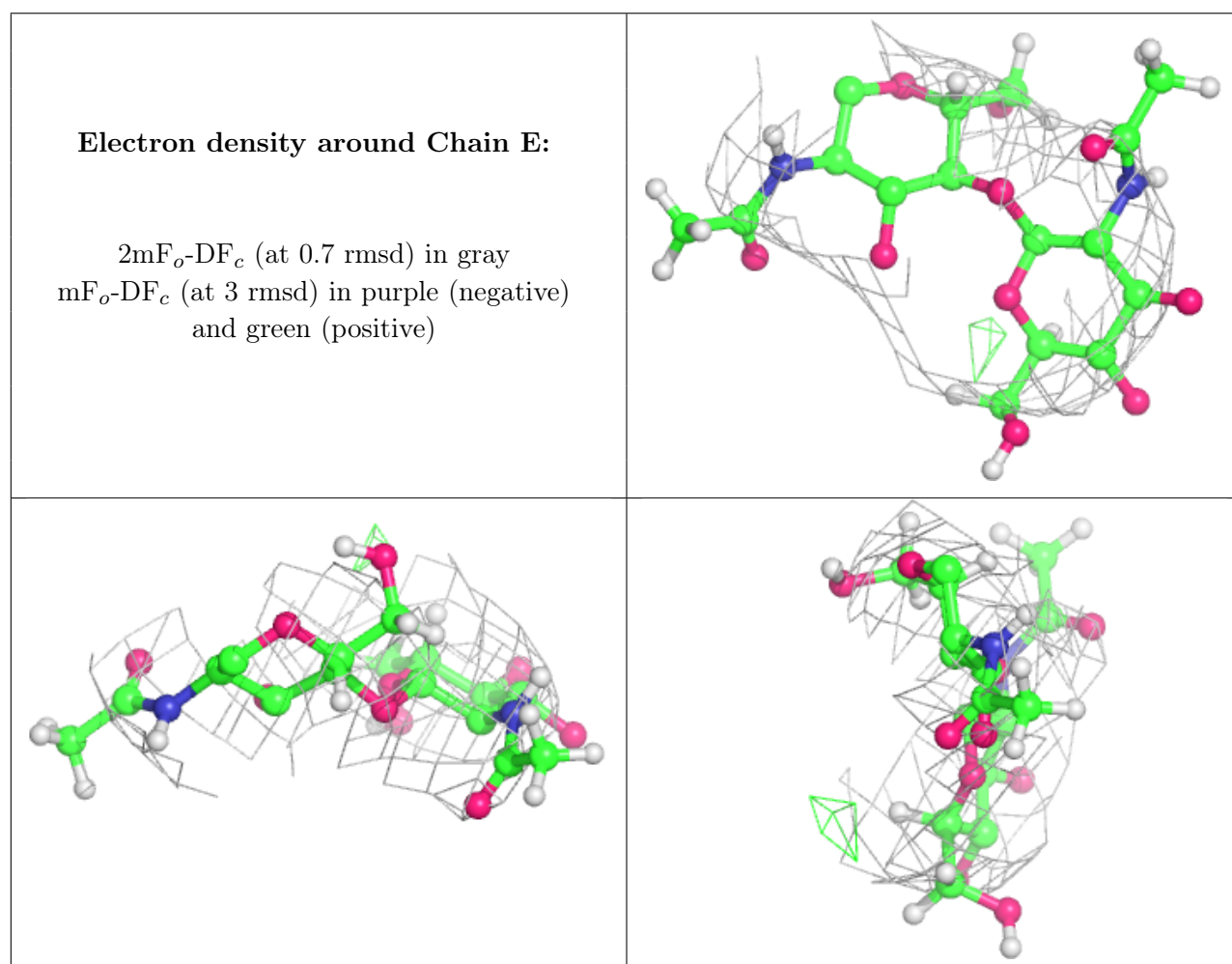
6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

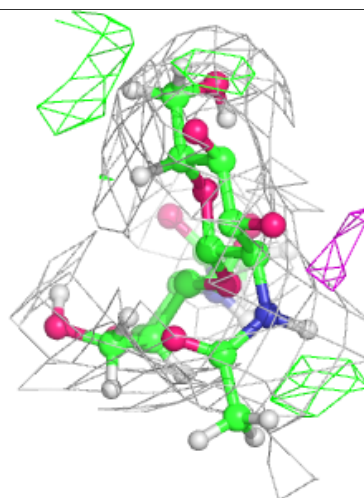
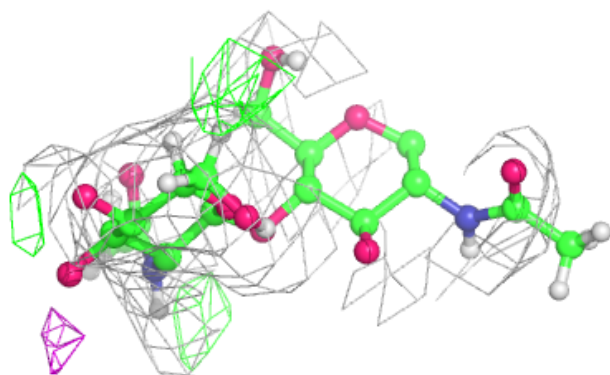
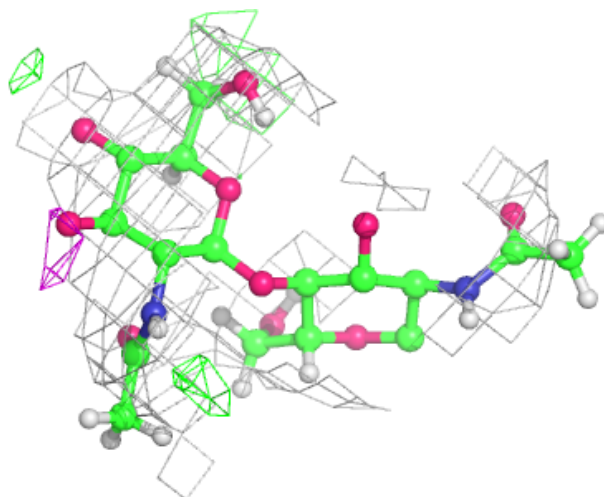
Unable to reproduce the depositors R factor - this section is therefore empty.

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.



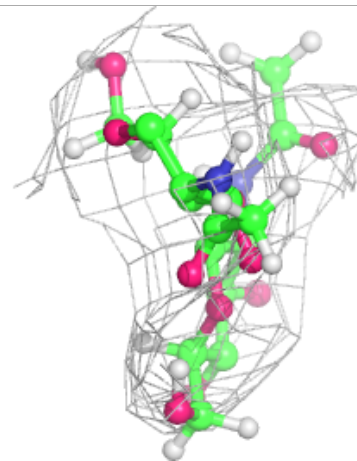
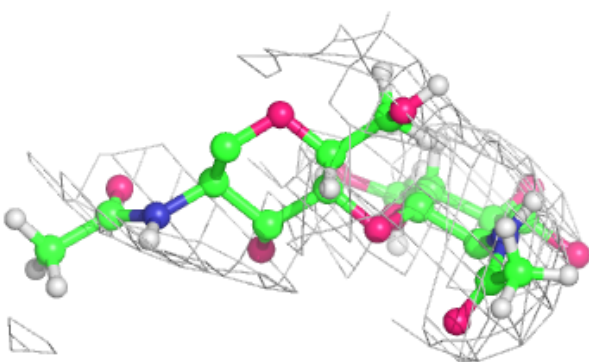
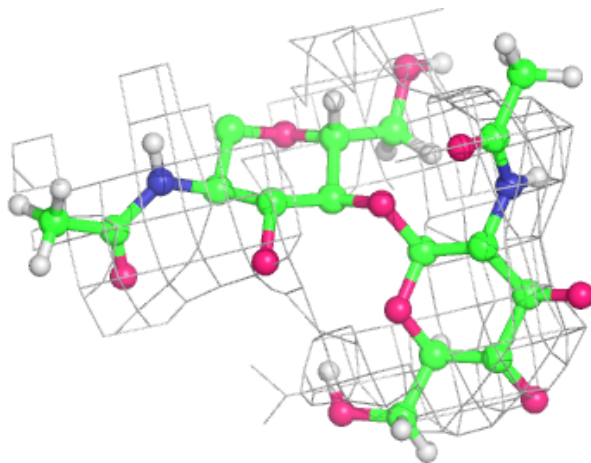
Electron density around Chain F:

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



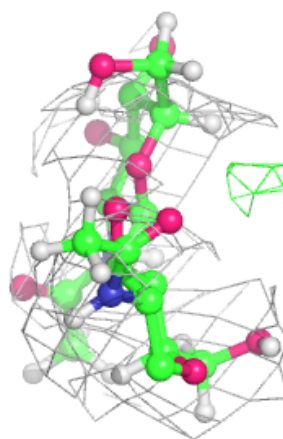
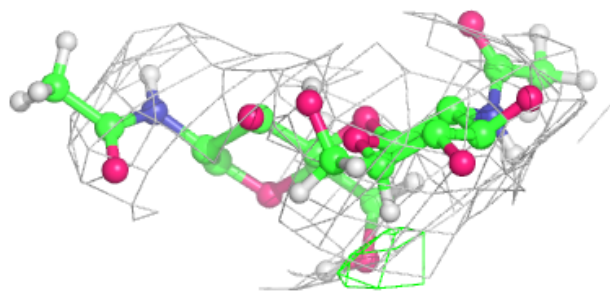
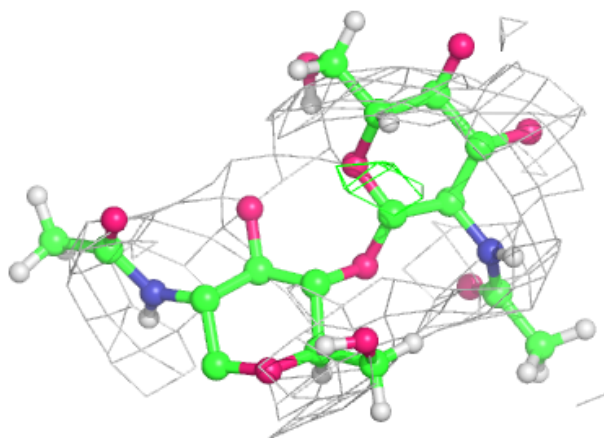
Electron density around Chain G:

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



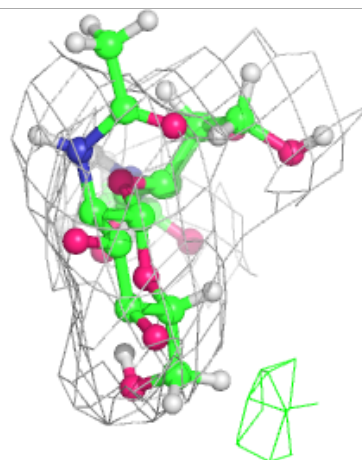
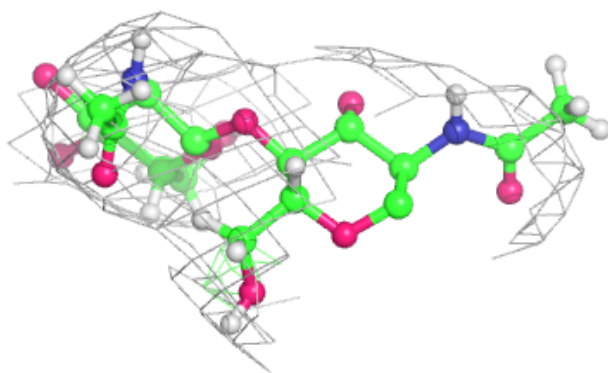
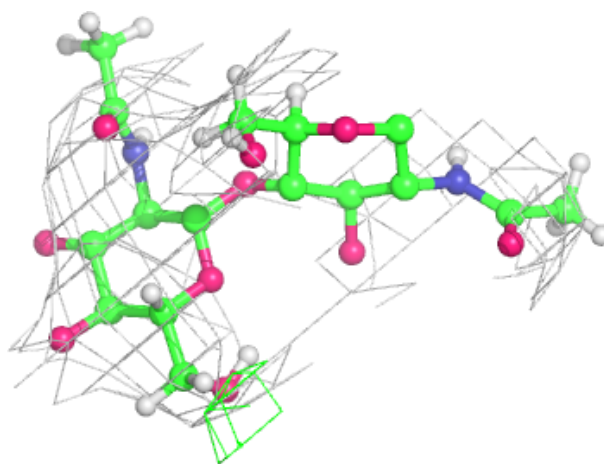
Electron density around Chain H:

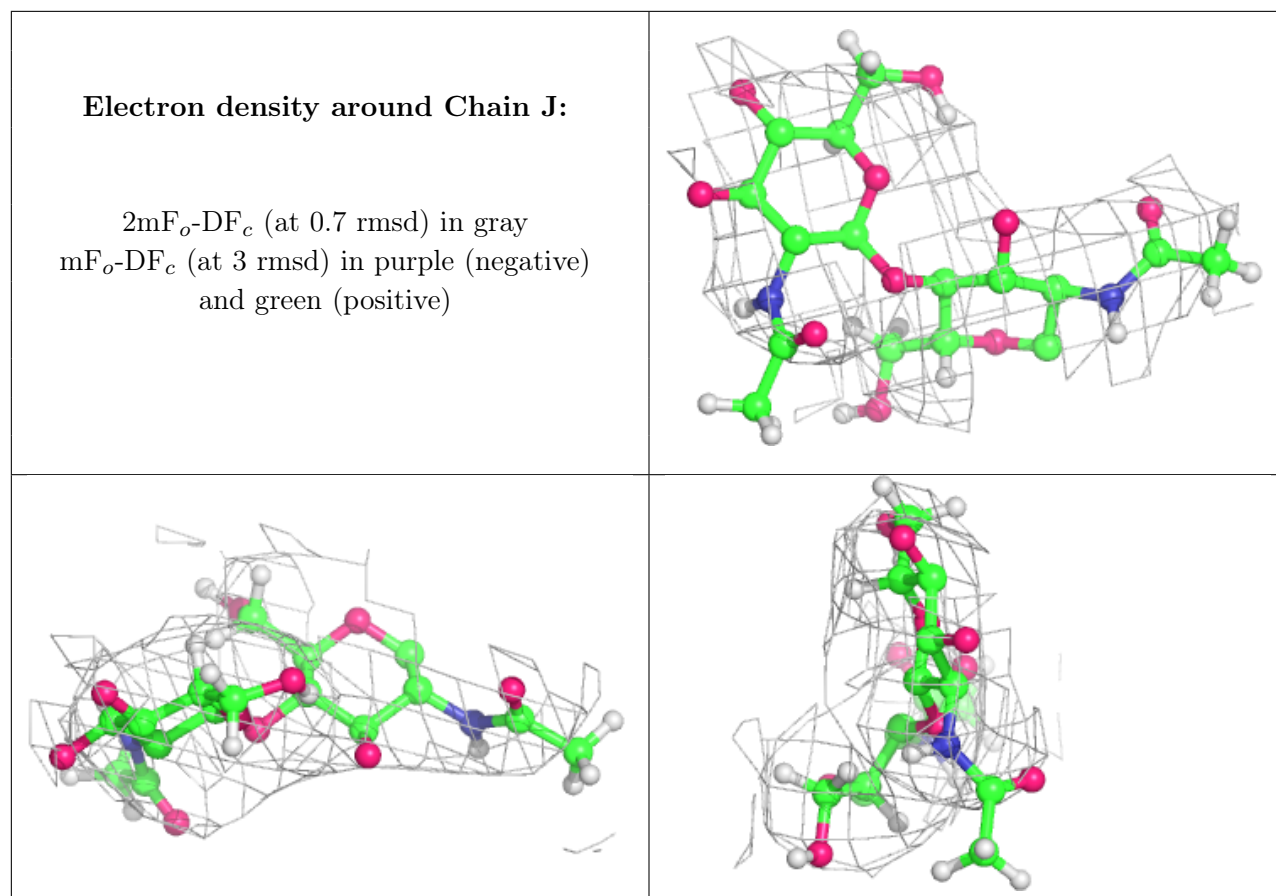
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain I:

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





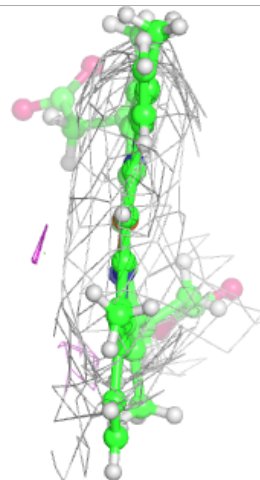
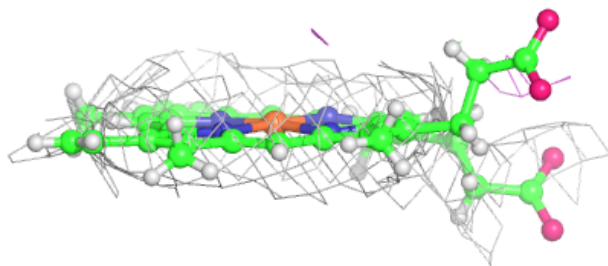
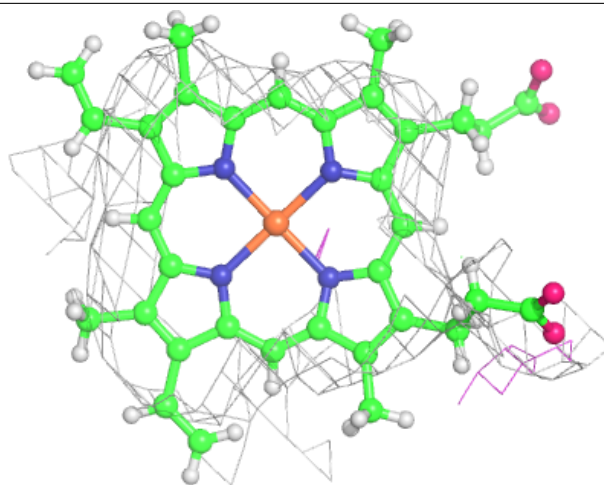
6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

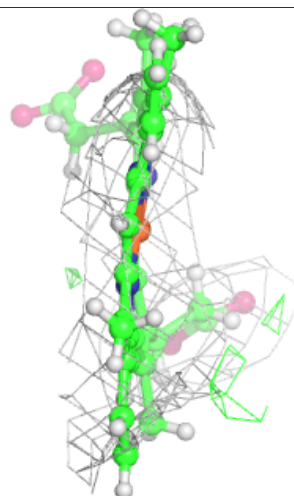
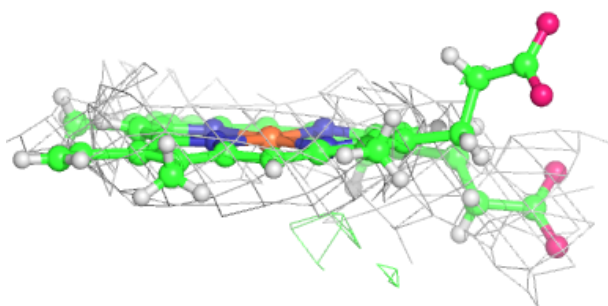
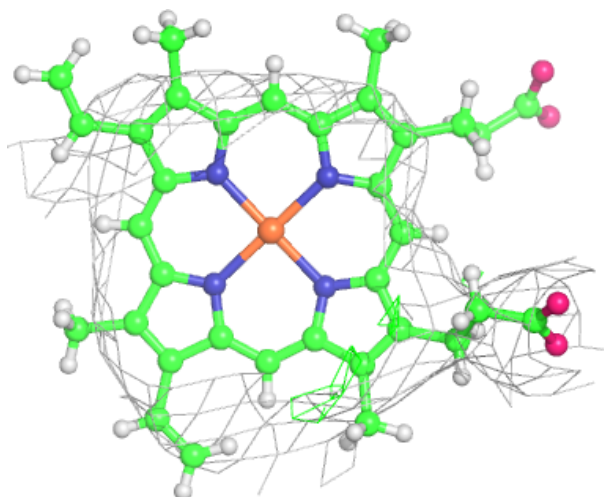
Electron density around HEM A 601:

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



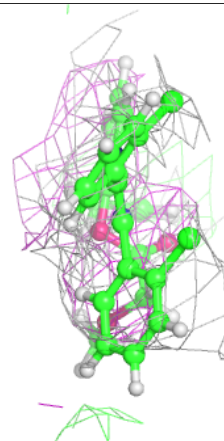
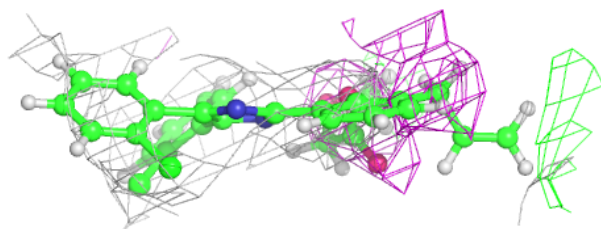
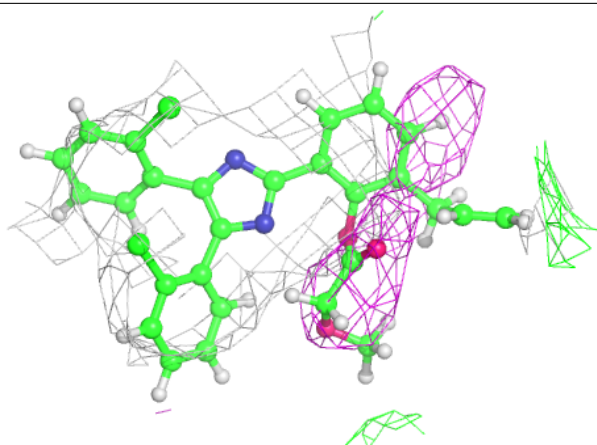
Electron density around HEM B 601:

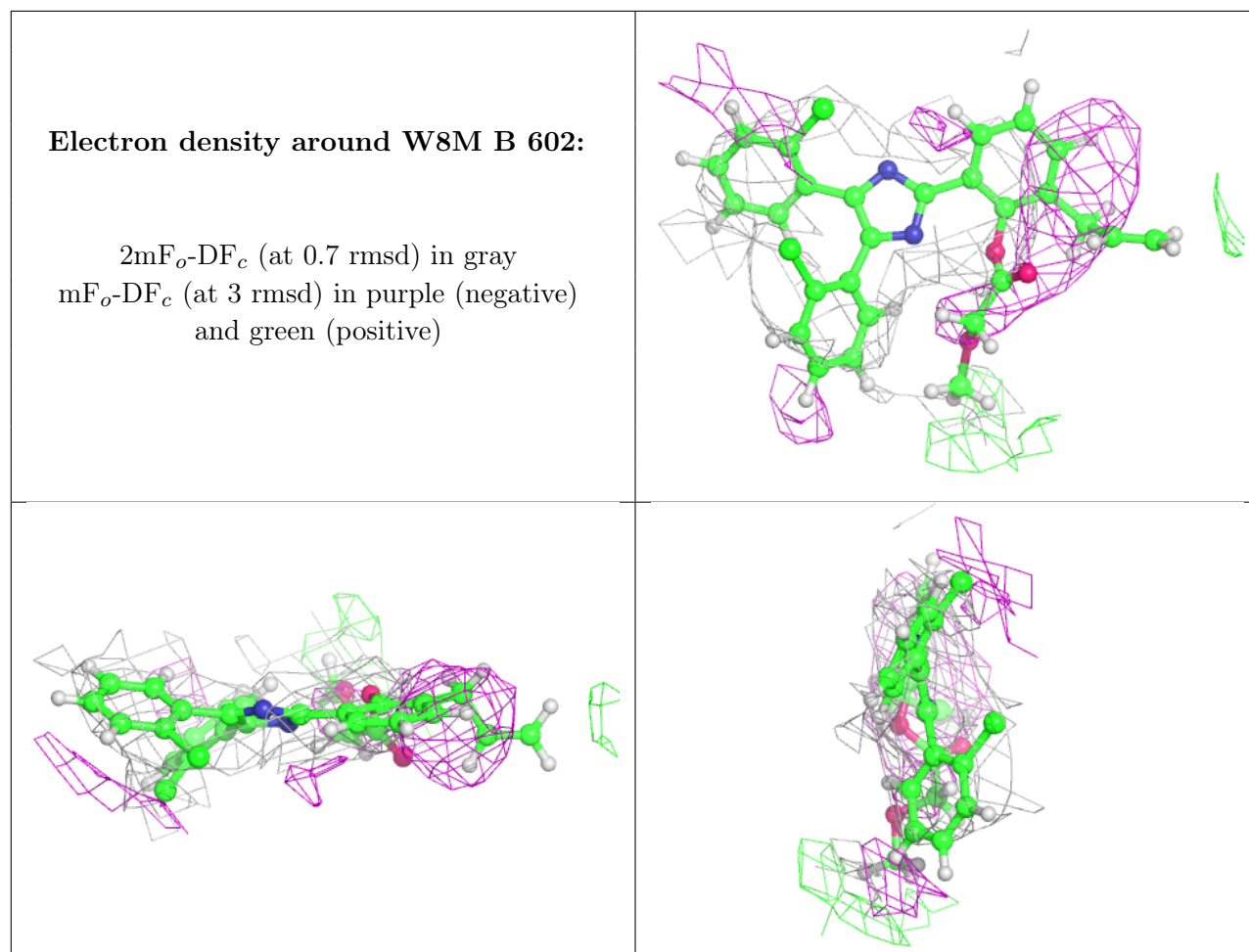
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around W8M A 602:

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





6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.