



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 02:28 AM EDT

PDB ID : 2YOR  
Title : Crystallization of a 45 kDa peroxygenase- peroxidase from the mushroom *Agrocybe aegerita* and structure determination by SAD utilizing only the haem iron  
Authors : Piontek, K.; Strittmatter, E.; Ullrich, R.; Plattner, D.A.; Hofrichter, M.  
Deposited on : 2012-10-26  
Resolution : 2.19 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

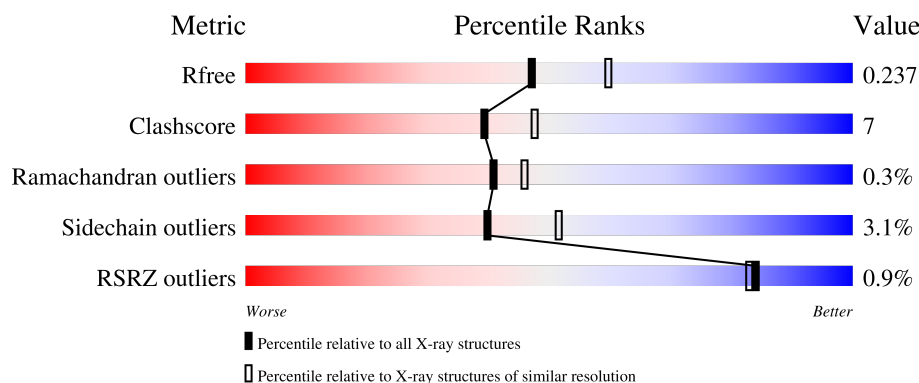
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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.



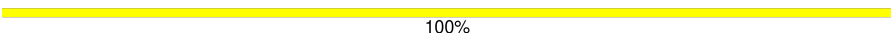
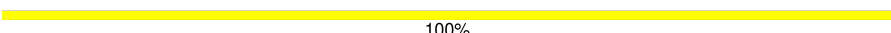
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	325	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>%</span> <span>89%</span> <span>10%</span> </div> </div>
1	B	325	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>%</span> <span>86%</span> <span>12%</span> </div> </div>
2	C	3	<div> <div style="display: flex; justify-content: space-between;"> <span>33%</span> <span>67%</span> </div> </div>
2	E	3	<div> <div style="display: flex; justify-content: space-between;"> <span>67%</span> <span>33%</span> </div> </div>
3	D	5	<div> <div style="display: flex; justify-content: space-between;"> <span>60%</span> <span>40%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
4	F	8	 12% 88%
5	G	2	 100%
5	H	2	 100%
5	I	2	 100%
5	J	2	 50% 50%

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
13	TRS	B	1355	-	-	-	X
2	BMA	C	3	-	-	-	X
2	BMA	E	3	-	-	-	X
4	MAN	F	6	-	-	-	X
5	NAG	H	2	-	-	-	X
5	NAG	I	2	-	-	-	X
5	NAG	J	1	X	-	-	X
5	NAG	J	2	-	-	-	X
9	NAG	A	401	-	-	-	X
9	NAG	B	411	-	-	-	X

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 6261 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 AROMATIC PEROXYGENASE.

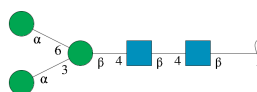
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2513	1590	438	477	8			
1	B	324	Total	C	N	O	S	0	2	0
			2521	1598	438	477	8			

- Molecule 2 is an oligosaccharide called 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
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

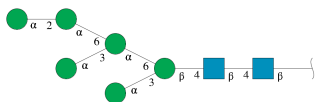
- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

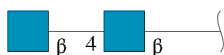
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyr

anose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



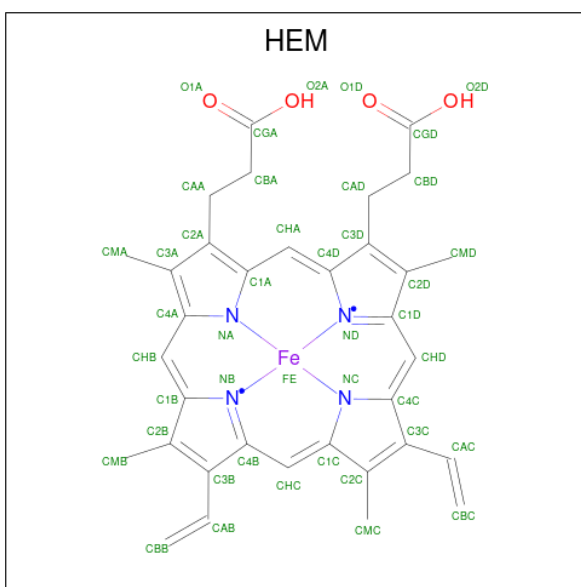
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 5 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
5	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).

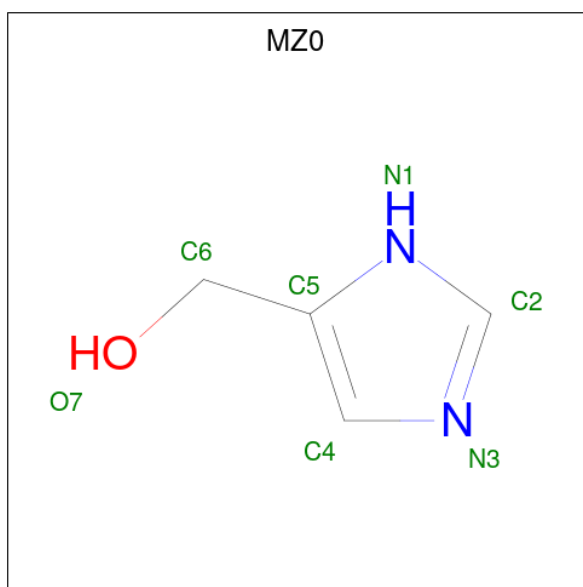


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 8 is 1H-imidazol-5-ylmethanol (three-letter code: MZ0) (formula:  $\text{C}_4\text{H}_6\text{N}_2\text{O}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			7	4	2	1		
8	B	1	Total	C	N	O	0	0
			7	4	2	1		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



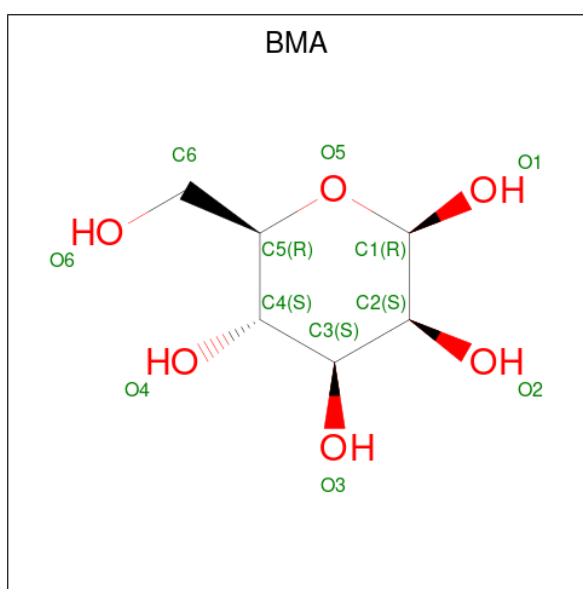
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 10 is beta-D-mannopyranose (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			12	6	6		
10	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 11 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



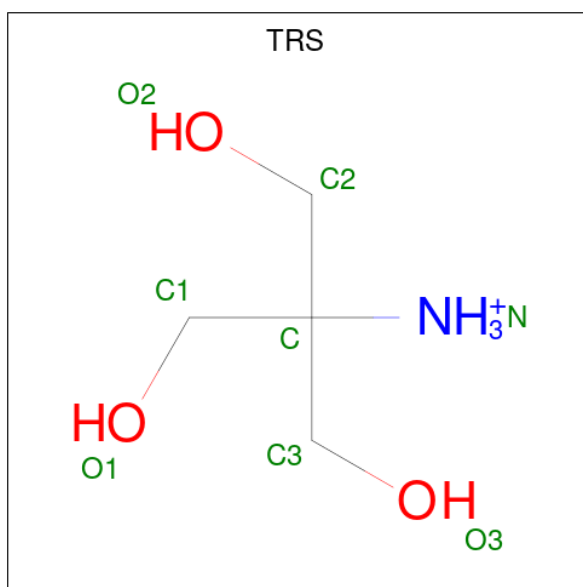


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total	Cl	0	0
			1	1		
12	B	3	Total	Cl	0	0
			3	3		

- Molecule 13 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	N	O	0	0
			8	4	1	3		

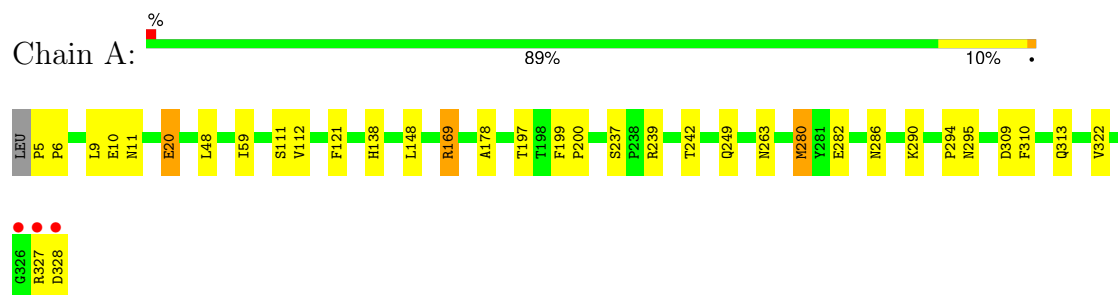
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	350	Total	O	0	0
			350	350		
14	B	293	Total	O	0	0
			293	293		

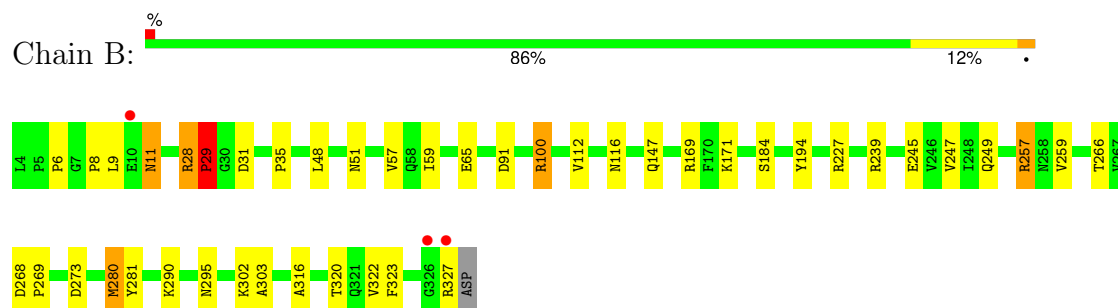
### 3 Residue-property plots [i](#)

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: AROMATIC PEROXYGENASE



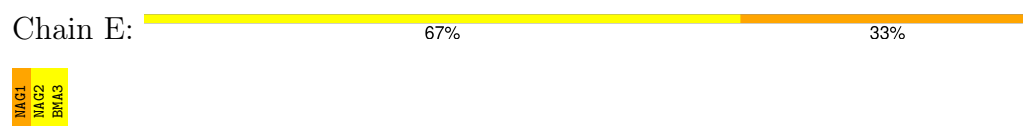
- Molecule 1: AROMATIC PEROXYGENASE



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



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



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

nose

Chain D:  60% 40%



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

Chain F:  12% 88%



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.29Å 95.03Å 127.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.51 – 2.19 47.52 – 2.19	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.51-2.19) 98.0 (47.52-2.19)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.46 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.169 , 0.237 0.170 , 0.237	Depositor DCC
$R_{free}$ test set	2384 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.6	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6261	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, MAN, SO4, NAG, MZ0, BMA, MG, CL, TRS

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	0.76	0/2583	0.70	1/3514 (0.0%)
1	B	0.75	0/2597	0.69	1/3535 (0.0%)
All	All	0.76	0/5180	0.70	2/7049 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	100	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	A	169	ARG	NE-CZ-NH1	-5.97	117.31	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	29	PRO	Peptide

### 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	2513	0	2387	27	0
1	B	2521	0	2404	37	0
2	C	39	0	34	2	0
2	E	39	0	34	1	0
3	D	61	0	52	2	0
4	F	94	0	79	0	0
5	G	28	0	25	0	0
5	H	28	0	25	0	0
5	I	28	0	25	0	0
5	J	28	0	25	2	0
6	A	43	0	30	4	0
6	B	43	0	30	2	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	7	0	6	0	0
8	B	7	0	6	0	0
9	A	42	0	38	6	0
9	B	29	0	28	4	0
10	A	12	0	12	3	0
10	B	12	0	12	3	0
11	A	15	0	0	0	0
11	B	15	0	0	1	0
12	A	1	0	0	0	0
12	B	3	0	0	1	0
13	B	8	0	12	1	0
14	A	350	0	0	5	0
14	B	293	0	0	8	0
All	All	6261	0	5264	80	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 7.

All (80) 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:B:303:ALA:HA	10:B:501:BMA:H62	1.35	1.04
6:A:350:HEM:HBC2	6:A:350:HEM:HMC2	1.44	0.95
1:A:294:PRO:HB2	9:A:401:NAG:H5	1.50	0.92
5:J:1:NAG:H4	5:J:2:NAG:N2	1.85	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:GLU:HG2	1:A:322:VAL:HG21	1.54	0.87
6:A:350:HEM:HBC2	6:A:350:HEM:CMC	2.09	0.81
1:B:295:ASN:HB2	14:B:2287:HOH:O	1.81	0.79
14:A:2336:HOH:O	2:E:1:NAG:H4	1.83	0.76
1:A:310:PHE:CE2	10:A:501:BMA:H4	2.21	0.75
1:B:280:MET:HE2	1:B:281:TYR:N	2.05	0.71
1:B:257:ARG:NH1	1:B:266:THR:O	2.23	0.71
1:B:259:VAL:HG12	1:B:259:VAL:O	1.92	0.70
11:B:1357:SO4:O3	14:B:2291:HOH:O	2.10	0.69
1:B:35:PRO:HD3	1:B:116:ASN:ND2	2.10	0.67
1:B:9:LEU:HD11	1:B:65:GLU:HG2	1.77	0.66
1:A:48:LEU:HD21	1:A:59:ILE:HA	1.76	0.66
1:B:303:ALA:CA	10:B:501:BMA:H62	2.18	0.66
1:B:227:ARG:HD2	14:B:2197:HOH:O	1.95	0.65
1:A:310:PHE:HE2	10:A:501:BMA:H4	1.63	0.62
6:A:350:HEM:HMC2	6:A:350:HEM:CBC	2.26	0.61
1:A:249:GLN:NE2	1:B:249:GLN:OE1	2.36	0.59
1:B:35:PRO:HD3	1:B:116:ASN:HD22	1.70	0.56
1:B:91:ASP:CG	10:B:501:BMA:H2	2.25	0.56
10:A:501:BMA:O1	14:A:2297:HOH:O	2.18	0.56
1:B:280:MET:O	1:B:280:MET:HE3	2.05	0.55
9:B:511:NAG:C6	14:B:2285:HOH:O	2.54	0.54
1:A:295:ASN:HB3	9:A:401:NAG:H83	1.89	0.54
14:A:2007:HOH:O	1:B:11:ASN:HA	2.08	0.54
1:A:327:ARG:O	1:A:328:ASP:O	2.26	0.54
9:B:511:NAG:H61	14:B:2285:HOH:O	2.07	0.53
1:B:227:ARG:CD	14:B:2197:HOH:O	2.53	0.53
1:B:11:ASN:C	1:B:11:ASN:OD1	2.47	0.53
1:B:280:MET:CE	1:B:280:MET:C	2.78	0.52
1:A:294:PRO:HG2	9:A:401:NAG:H3	1.90	0.52
1:B:184:SER:HB2	9:B:511:NAG:H4	1.91	0.52
1:A:294:PRO:CB	9:A:401:NAG:H5	2.32	0.52
2:C:2:NAG:C6	2:C:3:BMA:C1	2.89	0.51
1:A:295:ASN:HB2	9:A:401:NAG:N2	2.25	0.51
5:J:1:NAG:H4	5:J:2:NAG:C7	2.41	0.50
1:B:112:VAL:O	1:B:112:VAL:HG12	2.13	0.49
1:A:237:SER:HB3	1:B:8:PRO:HG3	1.95	0.48
1:A:309:ASP:O	1:A:313:GLN:HG2	2.13	0.48
1:A:112:VAL:HG12	1:A:112:VAL:O	2.13	0.48
1:A:282:GLU:HG2	1:A:322:VAL:CG2	2.36	0.48
1:B:245:GLU:OE2	14:B:2208:HOH:O	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3:BMA:H61	3:D:5:MAN:H5	1.94	0.47
1:B:9:LEU:CD1	1:B:65:GLU:HG2	2.42	0.47
2:C:2:NAG:H62	2:C:3:BMA:C1	2.44	0.47
3:D:3:BMA:H61	3:D:5:MAN:C5	2.44	0.47
1:A:242:THR:CG2	1:B:316:ALA:HB1	2.45	0.47
1:B:48:LEU:HD21	1:B:59:ILE:HA	1.96	0.46
6:B:350:HEM:CMC	6:B:350:HEM:HBC2	2.45	0.46
1:B:194:TYR:HD2	1:B:247:VAL:HG12	1.79	0.46
1:A:11:ASN:OD1	1:A:11:ASN:C	2.52	0.46
1:A:294:PRO:CG	9:A:401:NAG:H3	2.46	0.46
1:B:31:ASP:OD1	1:B:51:ASN:HA	2.16	0.46
1:B:302:LYS:HB3	1:B:302:LYS:HE2	1.51	0.46
9:B:511:NAG:H62	14:B:2285:HOH:O	2.16	0.46
1:A:138:HIS:HD2	14:A:2052:HOH:O	2.00	0.45
1:B:280:MET:HE3	1:B:280:MET:C	2.36	0.45
13:B:1355:TRS:O3	12:B:1358:CL:CL	2.72	0.45
1:A:5:PRO:HA	1:A:6:PRO:HD3	1.81	0.45
1:B:28:ARG:HA	1:B:29:PRO:HD2	1.72	0.45
1:A:282:GLU:O	1:A:286:ASN:HB2	2.17	0.44
6:B:350:HEM:HBC2	6:B:350:HEM:HMC1	1.98	0.44
1:A:169:ARG:HB2	1:A:197:THR:HG21	1.99	0.44
1:A:20:GLU:CD	1:A:20:GLU:H	2.20	0.44
1:B:322:VAL:CG2	1:B:323:PHE:N	2.80	0.44
1:A:148:LEU:HD23	1:A:148:LEU:C	2.38	0.44
1:A:280:MET:HE2	14:A:2277:HOH:O	2.18	0.43
6:A:350:HEM:HHC	6:A:350:HEM:CBB	2.48	0.43
1:B:268:ASP:HA	1:B:269:PRO:HD3	1.85	0.43
1:A:178:ALA:HA	1:A:263:ASN:ND2	2.33	0.43
1:B:280:MET:HE2	1:B:281:TYR:CA	2.48	0.43
1:B:28:ARG:O	1:B:28:ARG:HG3	2.20	0.42
1:B:273:ASP:C	1:B:273:ASP:OD1	2.57	0.42
1:B:280:MET:CE	1:B:281:TYR:N	2.79	0.42
1:A:199:PHE:N	1:A:200:PRO:CD	2.84	0.41
1:B:6:PRO:HD3	1:B:57:VAL:HG22	2.02	0.41
1:B:147:GLN:HE22	1:B:171:LYS:HE3	1.85	0.41

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	322/325 (99%)	307 (95%)	15 (5%)	0	100	100
1	B	324/325 (100%)	308 (95%)	14 (4%)	2 (1%)	25	26
All	All	646/650 (99%)	615 (95%)	29 (4%)	2 (0%)	41	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	PRO
1	B	11	ASN

### 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	270/271 (100%)	262 (97%)	8 (3%)	41	53
1	B	272/271 (100%)	263 (97%)	9 (3%)	38	49
All	All	542/542 (100%)	525 (97%)	17 (3%)	40	51

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	10	GLU
1	A	20	GLU
1	A	111	SER

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Mol	Chain	Res	Type
1	A	121	PHE
1	A	239	ARG
1	A	280	MET
1	A	290	LYS
1	B	28	ARG
1	B	100	ARG
1	B	169	ARG
1	B	239	ARG
1	B	257	ARG
1	B	280	MET
1	B	290	LYS
1	B	320	THR
1	B	327	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	116	ASN
1	A	263	ASN
1	A	307	ASN
1	A	313	GLN
1	B	71	ASN
1	B	116	ASN
1	B	147	GLN

### 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 ⓘ

27 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	0.64	0	17,19,21	1.31	4 (23%)
2	NAG	C	2	2	14,14,15	0.40	0	17,19,21	1.51	4 (23%)
2	BMA	C	3	2	11,11,12	0.47	0	15,15,17	1.17	2 (13%)
3	NAG	D	1	1,3	14,14,15	0.90	1 (7%)	17,19,21	1.55	4 (23%)
3	NAG	D	2	3	14,14,15	0.64	0	17,19,21	1.65	5 (29%)
3	BMA	D	3	3	11,11,12	0.59	0	15,15,17	1.40	3 (20%)
3	MAN	D	4	3	11,11,12	0.54	0	15,15,17	0.80	1 (6%)
3	MAN	D	5	3	11,11,12	0.55	0	15,15,17	0.85	1 (6%)
2	NAG	E	1	1,2	14,14,15	0.43	0	17,19,21	1.65	3 (17%)
2	NAG	E	2	2	14,14,15	0.64	0	17,19,21	1.26	1 (5%)
2	BMA	E	3	2	11,11,12	0.88	0	15,15,17	2.26	5 (33%)
4	NAG	F	1	1,4	14,14,15	0.83	0	17,19,21	1.40	4 (23%)
4	NAG	F	2	4	14,14,15	0.86	0	17,19,21	1.06	1 (5%)
4	BMA	F	3	4	11,11,12	0.61	0	15,15,17	1.04	1 (6%)
4	MAN	F	4	4	11,11,12	0.58	0	15,15,17	1.01	1 (6%)
4	MAN	F	5	4	11,11,12	0.51	0	15,15,17	1.31	2 (13%)
4	MAN	F	6	4	11,11,12	0.71	0	15,15,17	1.55	3 (20%)
4	MAN	F	7	4	11,11,12	0.42	0	15,15,17	1.41	3 (20%)
4	MAN	F	8	4	11,11,12	0.63	0	15,15,17	0.93	0
5	NAG	G	1	1,5	14,14,15	0.78	0	17,19,21	1.79	6 (35%)
5	NAG	G	2	5	14,14,15	0.64	0	17,19,21	2.06	3 (17%)
5	NAG	H	1	1,5	14,14,15	0.78	0	17,19,21	1.54	2 (11%)
5	NAG	H	2	5	14,14,15	0.53	0	17,19,21	1.94	3 (17%)
5	NAG	I	1	1,5	14,14,15	0.58	0	17,19,21	2.59	6 (35%)
5	NAG	I	2	5	14,14,15	0.52	0	17,19,21	1.26	2 (11%)
5	NAG	J	1	1,5	14,14,15	0.50	0	17,19,21	1.01	1 (5%)
5	NAG	J	2	5	14,14,15	0.69	0	17,19,21	0.74	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	1/1/1/1
3	MAN	D	5	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	MAN	F	6	4	-	2/2/19/22	0/1/1/1
4	MAN	F	7	4	-	0/2/19/22	0/1/1/1
4	MAN	F	8	4	-	0/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	4/6/23/26	0/1/1/1
5	NAG	H	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	NAG	J	1	1,5	1/1/5/7	1/6/23/26	0/1/1/1
5	NAG	J	2	5	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	C1-C2	2.37	1.55	1.52

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1	NAG	C4-C3-C2	-6.09	102.09	111.02
5	G	2	NAG	C1-O5-C5	-5.93	104.24	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	2	NAG	C1-O5-C5	5.63	119.72	112.19
2	E	3	BMA	C3-C4-C5	-4.84	101.45	110.23
5	I	1	NAG	O4-C4-C3	4.77	121.62	110.38
5	H	1	NAG	C4-C3-C2	4.67	117.86	111.02
5	I	1	NAG	O4-C4-C5	4.47	120.34	109.32
2	E	2	NAG	C4-C3-C2	4.33	117.36	111.02
2	E	1	NAG	C1-O5-C5	4.07	117.64	112.19
4	F	6	MAN	C1-C2-C3	3.89	115.30	109.64
2	E	3	BMA	C2-C3-C4	-3.87	104.05	110.86
5	G	1	NAG	O4-C4-C3	-3.61	101.87	110.38
4	F	5	MAN	C1-C2-C3	-3.50	104.55	109.64
5	H	2	NAG	C4-C3-C2	-3.49	105.91	111.02
3	D	2	NAG	O5-C5-C6	3.47	114.42	107.66
3	D	3	BMA	C1-O5-C5	3.46	116.82	112.19
5	I	2	NAG	C2-N2-C7	-3.44	118.28	122.90
2	E	1	NAG	C3-C4-C5	-3.42	104.03	110.23
5	G	2	NAG	O5-C1-C2	-3.38	106.06	111.29
5	G	2	NAG	C4-C3-C2	3.37	115.96	111.02
2	C	2	NAG	O4-C4-C3	-3.36	102.46	110.38
4	F	7	MAN	C1-O5-C5	3.31	116.62	112.19
2	E	3	BMA	O5-C5-C6	3.21	113.91	107.66
5	I	1	NAG	C1-C2-N2	3.13	115.36	110.43
4	F	6	MAN	C2-C3-C4	3.07	116.27	110.86
5	G	1	NAG	O5-C1-C2	-3.03	106.60	111.29
3	D	1	NAG	C6-C5-C4	-3.03	105.59	113.02
5	I	2	NAG	O5-C1-C2	-3.00	106.64	111.29
3	D	3	BMA	C1-C2-C3	3.00	114.01	109.64
3	D	2	NAG	C1-O5-C5	-2.97	108.21	112.19
4	F	1	NAG	O5-C1-C2	-2.96	106.71	111.29
2	C	2	NAG	C1-O5-C5	2.71	115.82	112.19
2	C	1	NAG	C4-C3-C2	2.69	114.95	111.02
3	D	1	NAG	O4-C4-C3	2.64	116.60	110.38
5	I	1	NAG	O5-C5-C4	-2.62	104.47	110.83
5	G	1	NAG	C4-C3-C2	2.60	114.83	111.02
4	F	1	NAG	C1-O5-C5	2.53	115.58	112.19
3	D	2	NAG	C2-N2-C7	-2.52	119.53	122.90
5	J	1	NAG	O5-C1-C2	2.50	115.15	111.29
2	C	2	NAG	O4-C4-C5	2.49	115.46	109.32
2	E	3	BMA	O3-C3-C2	2.49	115.14	110.05
2	E	3	BMA	O2-C2-C3	-2.47	105.03	110.15
2	C	1	NAG	O5-C1-C2	-2.46	107.49	111.29
3	D	2	NAG	C4-C3-C2	2.40	114.54	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	3	BMA	O2-C2-C1	2.37	114.65	109.22
4	F	7	MAN	C6-C5-C4	-2.35	107.24	113.02
5	G	1	NAG	C1-O5-C5	2.34	115.32	112.19
5	H	2	NAG	O5-C1-C2	2.29	114.83	111.29
3	D	4	MAN	C1-O5-C5	2.27	115.22	112.19
4	F	4	MAN	C2-C3-C4	-2.24	106.93	110.86
2	C	2	NAG	C3-C4-C5	-2.22	106.21	110.23
4	F	6	MAN	C3-C4-C5	2.21	114.24	110.23
4	F	7	MAN	C2-C3-C4	-2.19	107.02	110.86
2	C	3	BMA	C1-C2-C3	2.18	112.81	109.64
2	C	3	BMA	C1-O5-C5	2.18	115.10	112.19
3	D	5	MAN	C1-C2-C3	2.17	112.80	109.64
2	C	1	NAG	C2-N2-C7	-2.16	120.00	122.90
5	I	1	NAG	C3-C4-C5	2.15	114.13	110.23
3	D	2	NAG	C3-C4-C5	-2.14	106.35	110.23
4	F	1	NAG	O3-C3-C4	-2.12	105.38	110.38
5	G	1	NAG	C1-C2-N2	2.12	113.77	110.43
3	D	1	NAG	C4-C3-C2	-2.10	107.94	111.02
5	H	1	NAG	C3-C4-C5	2.08	114.01	110.23
3	D	3	BMA	C3-C4-C5	2.08	114.00	110.23
5	G	1	NAG	C2-N2-C7	-2.07	120.13	122.90
2	C	1	NAG	O4-C4-C3	-2.06	105.52	110.38
2	E	1	NAG	O4-C4-C3	-2.04	105.56	110.38
4	F	5	MAN	O5-C5-C6	2.04	111.63	107.66
4	F	2	NAG	C1-O5-C5	2.03	114.91	112.19
3	D	1	NAG	C1-O5-C5	2.00	114.87	112.19
4	F	1	NAG	O5-C5-C4	-2.00	105.95	110.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	J	1	NAG	C1

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	2	NAG	C1-C2-N2-C7
2	C	3	BMA	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	F	6	MAN	C4-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
4	F	6	MAN	O5-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
3	D	5	MAN	C4-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
3	D	5	MAN	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
5	J	1	NAG	C1-C2-N2-C7
4	F	3	BMA	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	4	MAN	C1-C2-C3-C4-C5-O5

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0
5	J	1	NAG	2	0
2	C	3	BMA	2	0
2	C	2	NAG	2	0

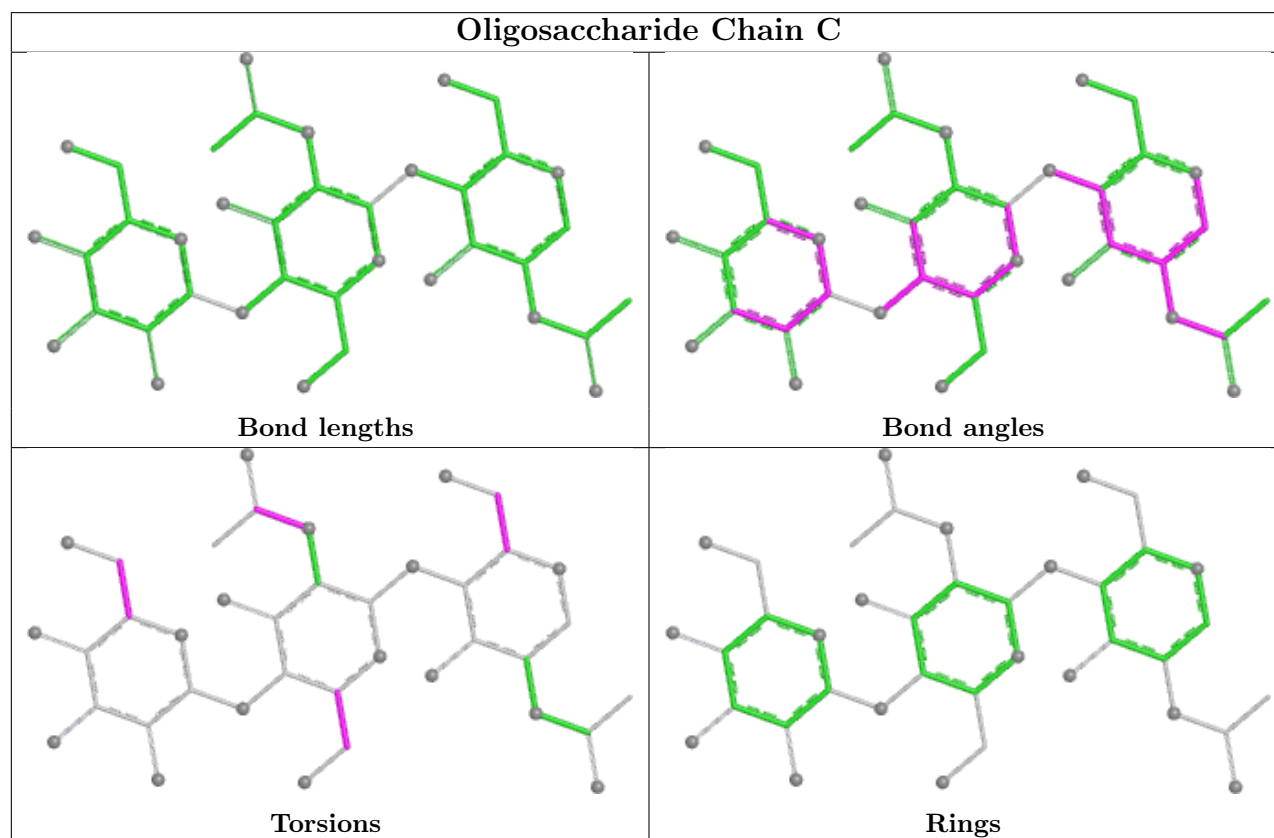
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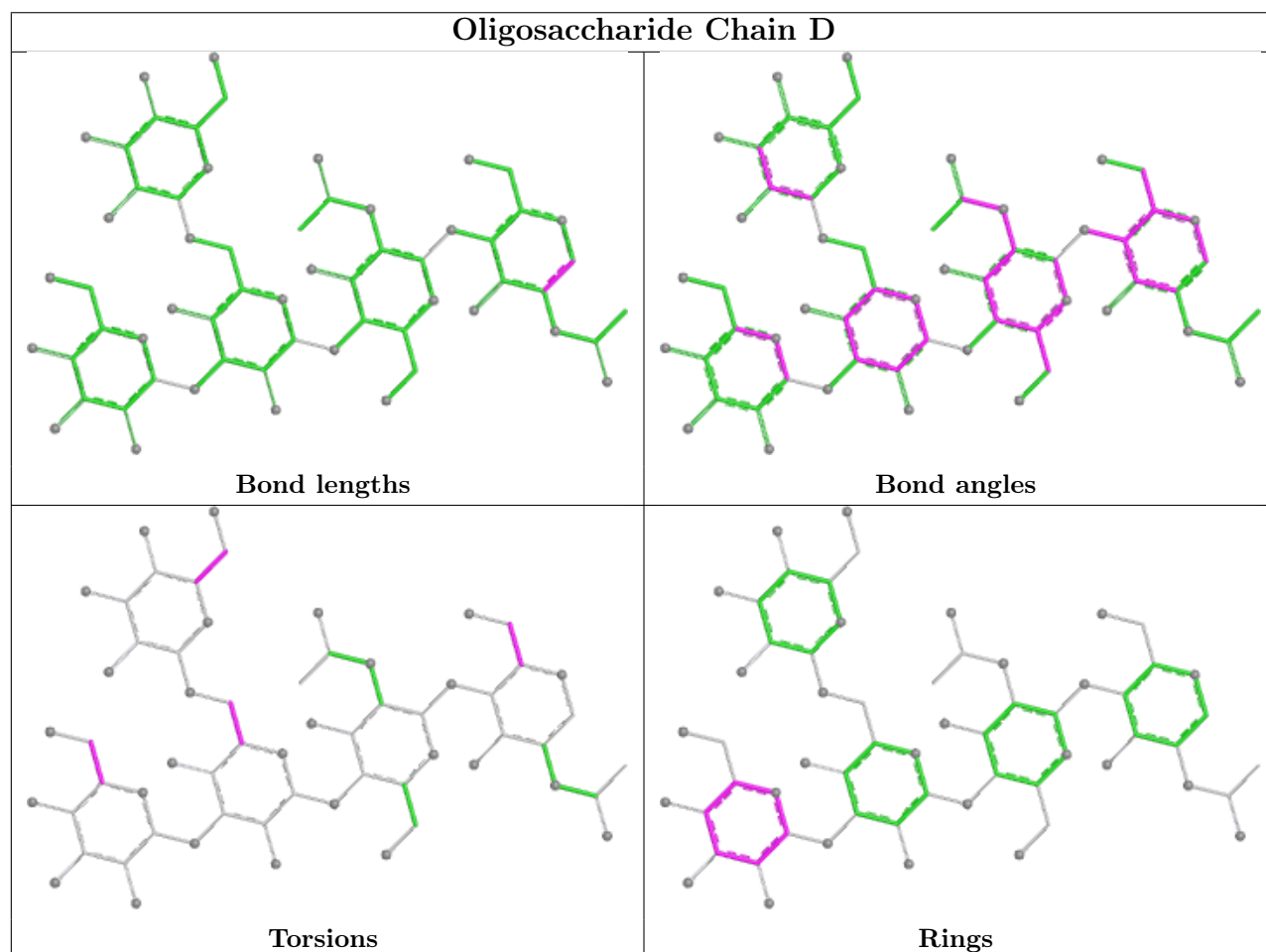
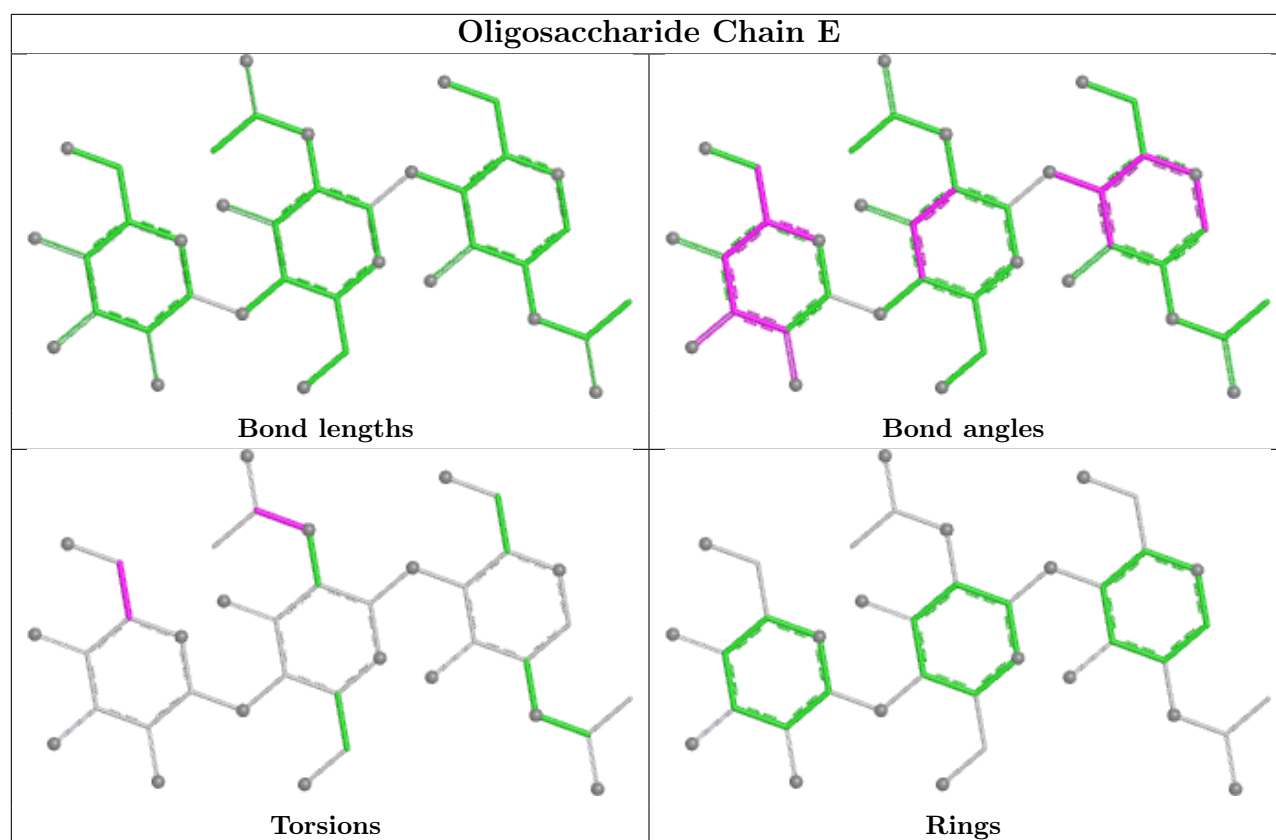


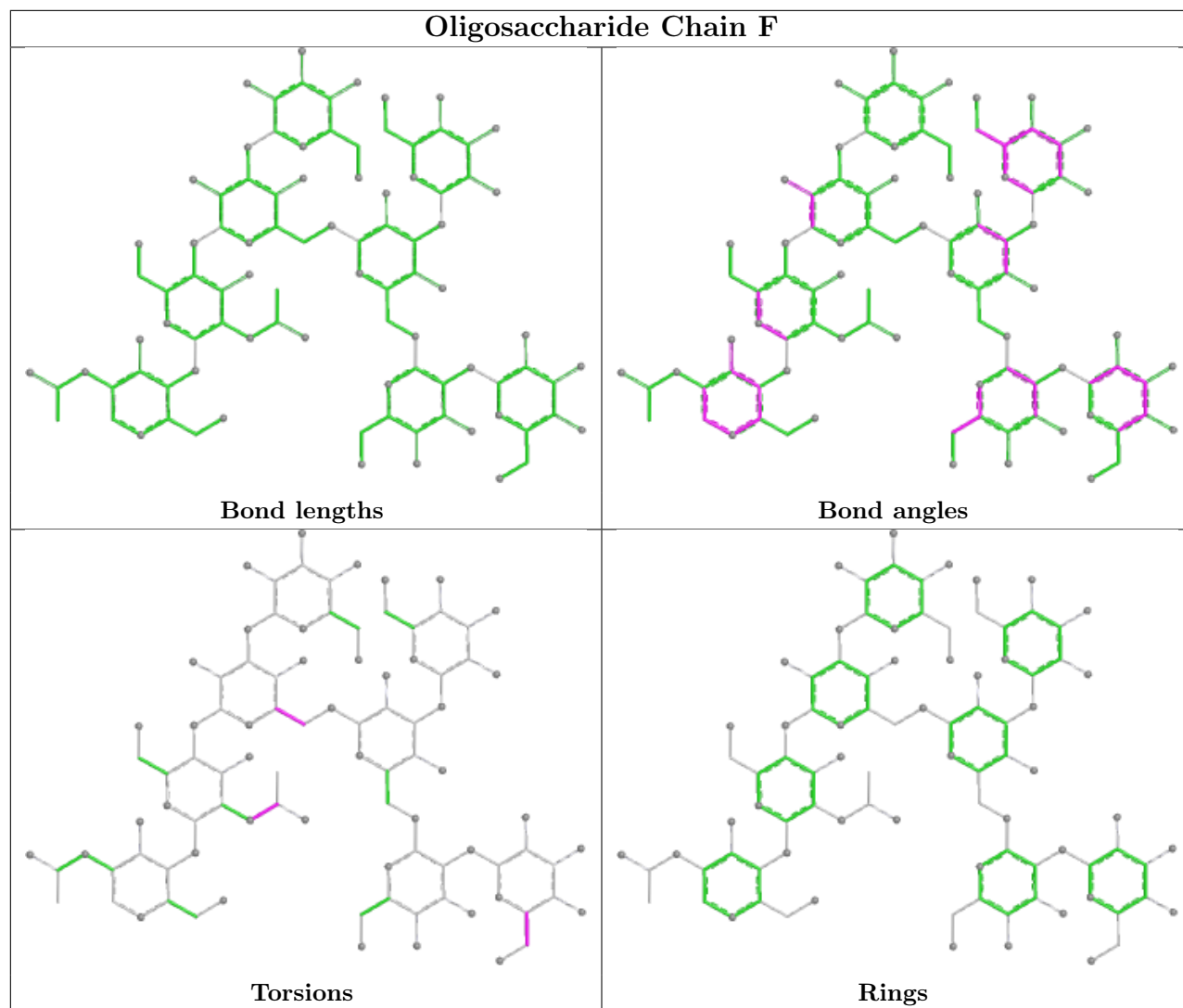
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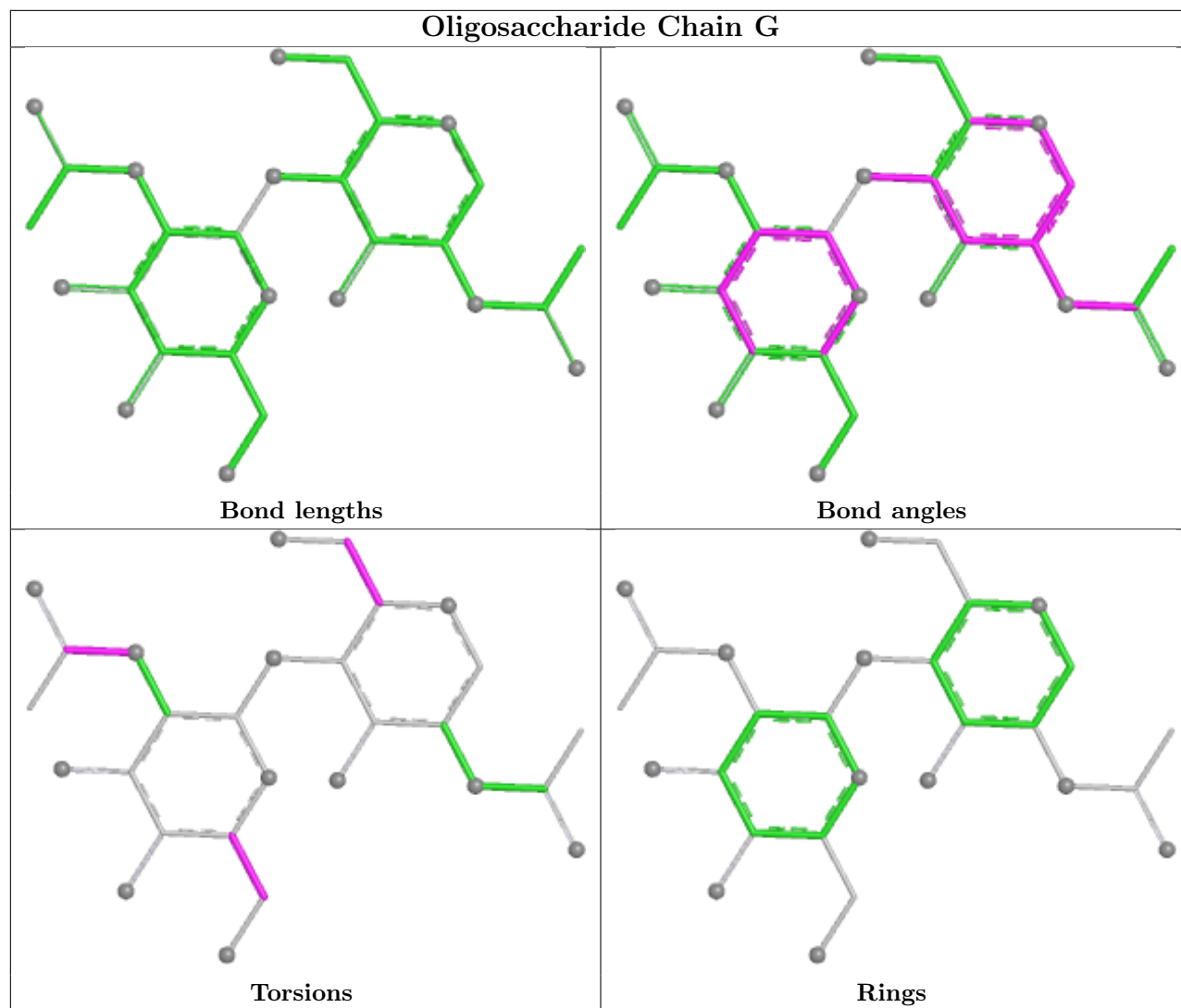
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	5	MAN	2	0
5	J	2	NAG	2	0
3	D	3	BMA	2	0

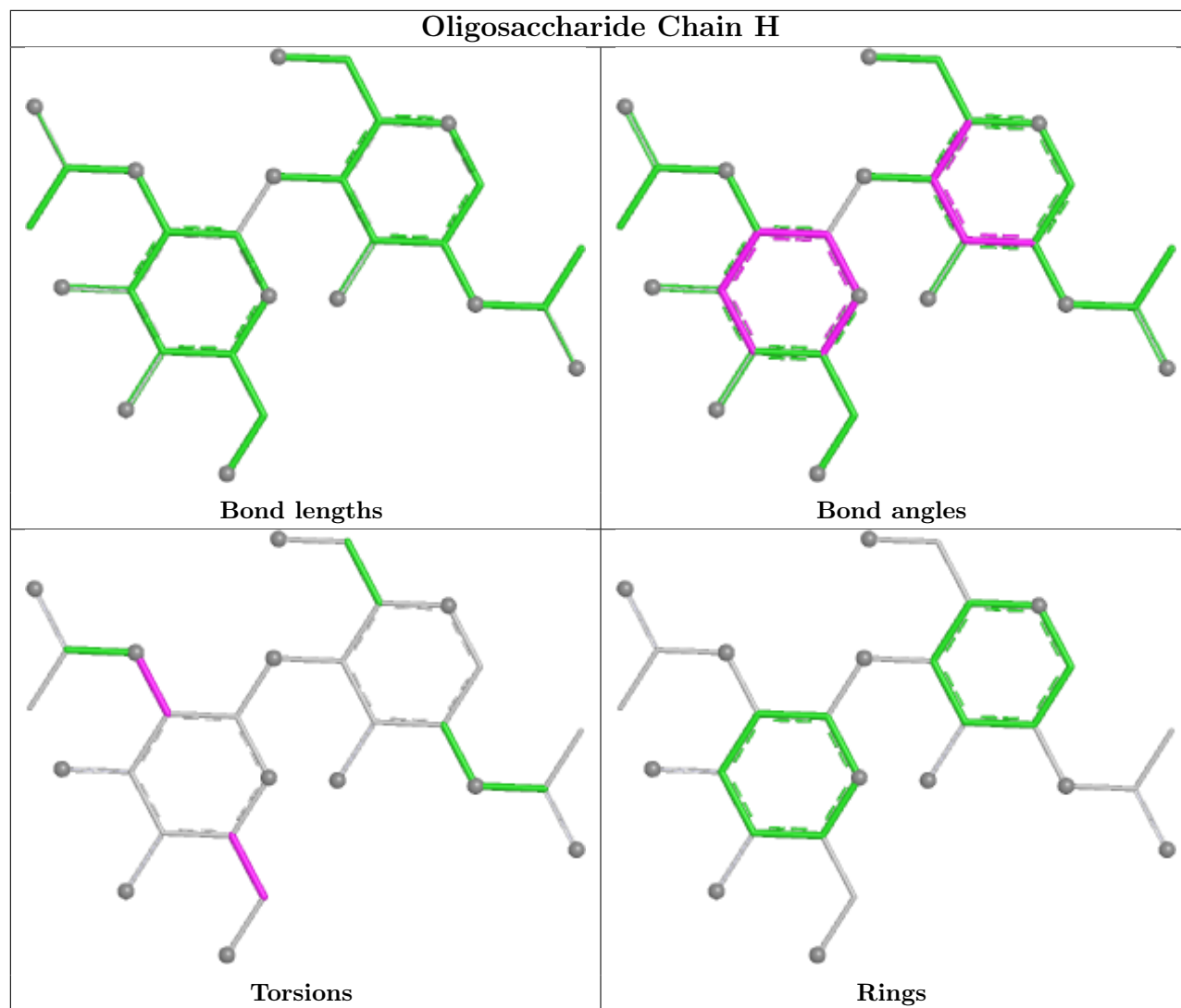
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

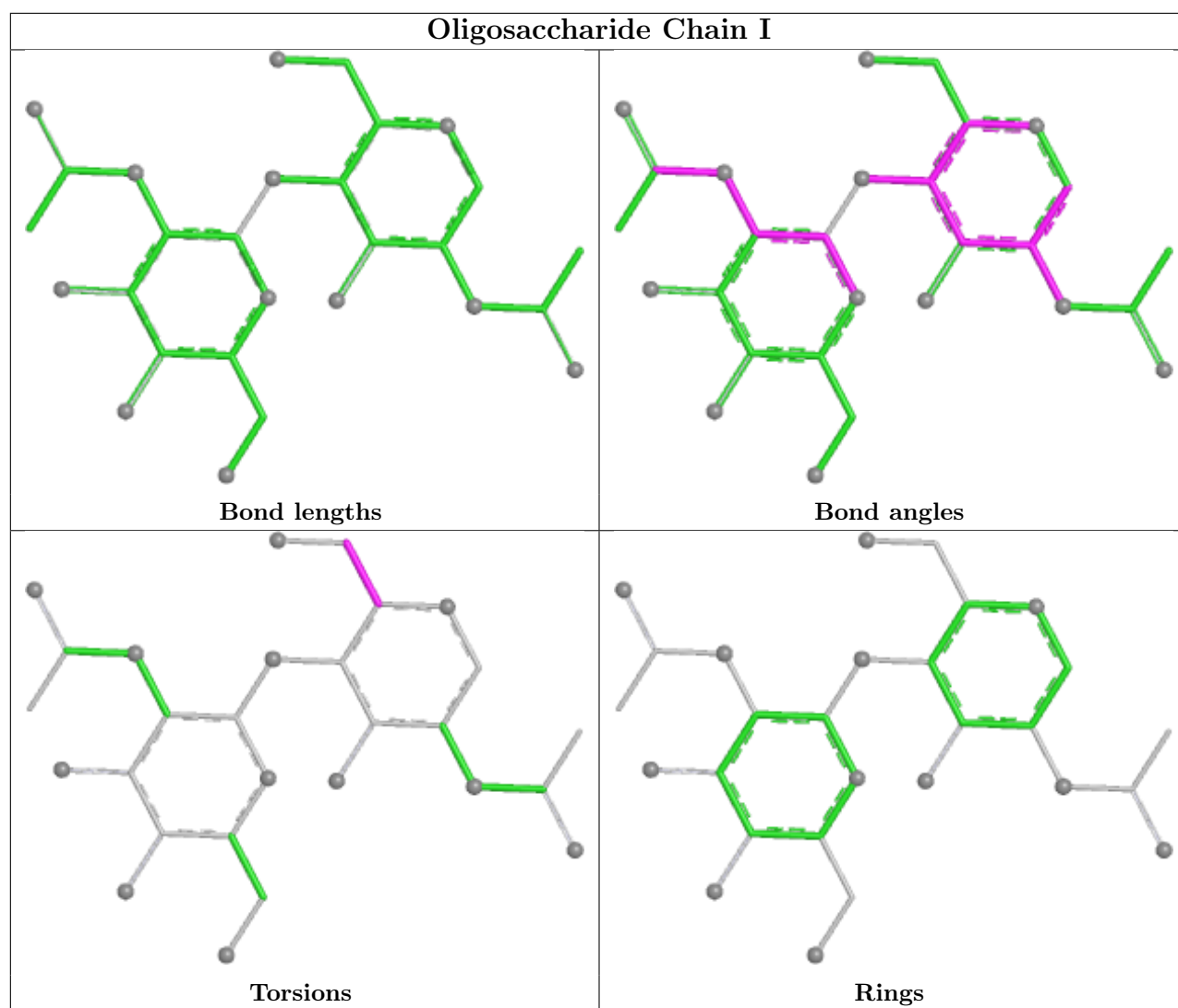


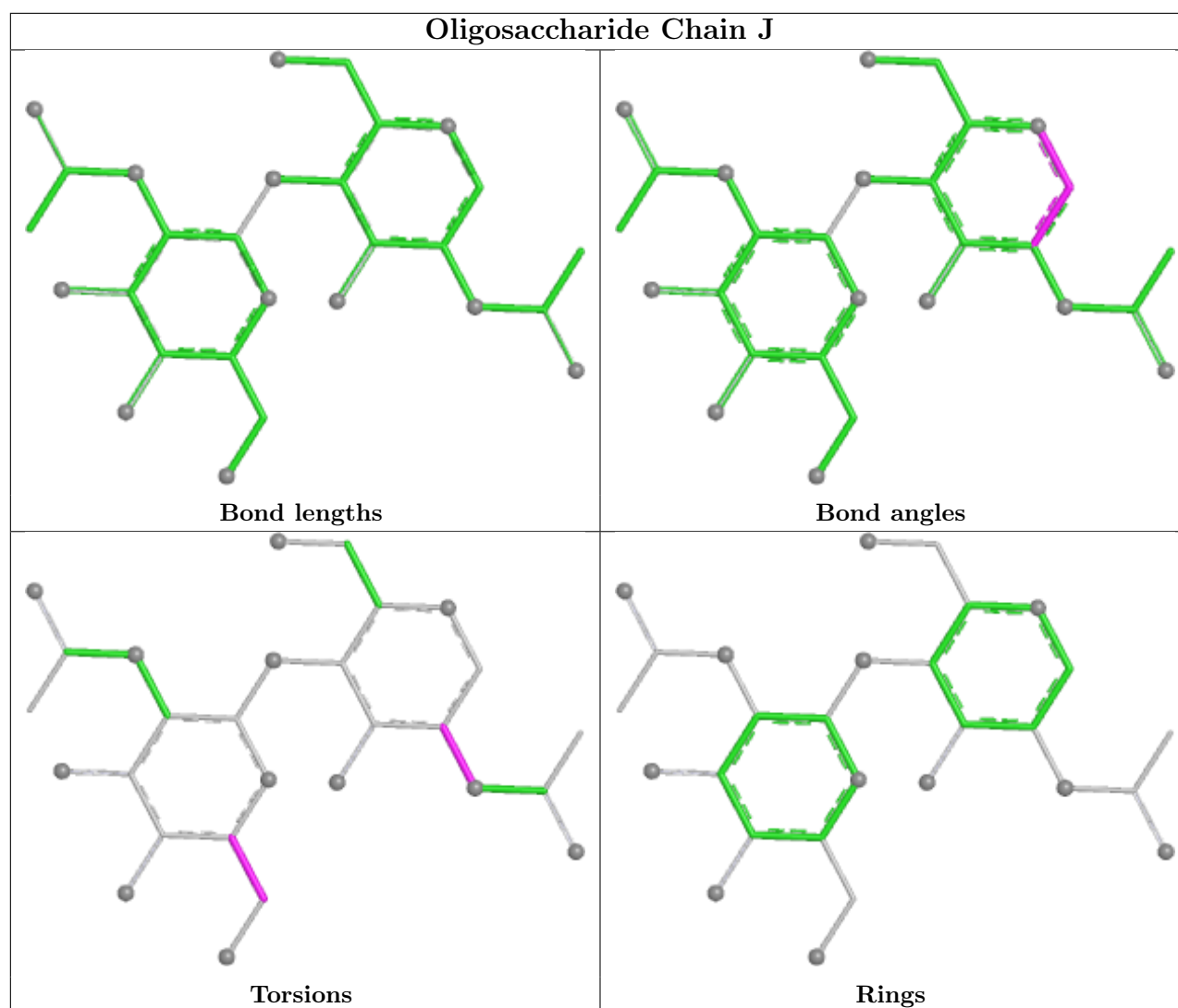












## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
9	NAG	A	391	1	14,14,15	0.55	0	17,19,21	0.62	0
13	TRS	B	1355	-	7,7,7	0.32	0	9,9,9	0.33	0
11	SO4	A	1357	-	4,4,4	0.27	0	6,6,6	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	SO4	A	1358	-	4,4,4	0.23	0	6,6,6	0.05	0
11	SO4	A	1355	-	4,4,4	0.23	0	6,6,6	0.08	0
9	NAG	B	511	-	15,15,15	0.81	1 (6%)	21,21,21	2.22	8 (38%)
11	SO4	B	1357	-	4,4,4	0.26	0	6,6,6	0.28	0
8	MZ0	A	354	6	3,7,7	0.53	0	4,8,8	1.24	0
8	MZ0	B	354	6	3,7,7	0.46	0	4,8,8	1.11	0
9	NAG	B	411	1	14,14,15	0.53	0	17,19,21	0.76	0
11	SO4	B	1360	-	4,4,4	0.28	0	6,6,6	0.26	0
6	HEM	A	350	1,7,8	42,50,50	1.85	10 (23%)	46,82,82	1.66	13 (28%)
6	HEM	B	350	1,7,8	42,50,50	1.80	8 (19%)	46,82,82	1.44	8 (17%)
9	NAG	A	411	1	14,14,15	1.56	3 (21%)	17,19,21	2.04	5 (29%)
9	NAG	A	401	1	14,14,15	0.58	0	17,19,21	3.68	4 (23%)
11	SO4	B	1359	-	4,4,4	0.26	0	6,6,6	0.26	0
10	BMA	A	501	-	12,12,12	0.91	0	17,17,17	1.97	5 (29%)
10	BMA	B	501	-	12,12,12	0.69	0	17,17,17	1.45	2 (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
9	NAG	A	391	1	-	2/6/23/26	0/1/1/1
13	TRS	B	1355	-	-	9/9/9/9	-
9	NAG	B	511	-	-	0/6/26/26	0/1/1/1
8	MZ0	A	354	6	-	0/0/2/2	0/1/1/1
8	MZ0	B	354	6	-	0/0/2/2	0/1/1/1
9	NAG	B	411	1	-	2/6/23/26	0/1/1/1
6	HEM	A	350	1,7,8	-	2/12/54/54	-
6	HEM	B	350	1,7,8	-	2/12/54/54	-
9	NAG	A	411	1	-	2/6/23/26	0/1/1/1
9	NAG	A	401	1	-	4/6/23/26	0/1/1/1
10	BMA	A	501	-	-	2/2/22/22	0/1/1/1
10	BMA	B	501	-	-	2/2/22/22	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	350	HEM	C3D-C2D	5.90	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	350	HEM	C3C-C2C	-5.76	1.32	1.40
6	A	350	HEM	C3D-C2D	5.65	1.49	1.36
6	B	350	HEM	C3C-C2C	-5.58	1.32	1.40
9	A	411	NAG	O5-C1	-3.27	1.38	1.43
6	A	350	HEM	C3C-CAC	3.09	1.54	1.47
6	A	350	HEM	CMA-C3A	3.05	1.57	1.51
6	B	350	HEM	C3C-CAC	2.92	1.54	1.47
6	A	350	HEM	CMB-C2B	2.85	1.56	1.50
6	B	350	HEM	CMB-C2B	2.77	1.56	1.50
6	B	350	HEM	C3B-C2B	-2.64	1.31	1.37
9	A	411	NAG	C2-N2	-2.57	1.42	1.46
6	A	350	HEM	CMC-C2C	2.50	1.57	1.51
9	A	411	NAG	C1-C2	-2.38	1.49	1.52
6	B	350	HEM	CMC-C2C	2.23	1.56	1.51
6	A	350	HEM	C3B-C2B	-2.20	1.32	1.37
6	B	350	HEM	CAB-C3B	2.14	1.53	1.47
6	B	350	HEM	CMD-C2D	2.12	1.55	1.50
9	B	511	NAG	C1-C2	2.10	1.55	1.52
6	A	350	HEM	O1D-CGD	2.05	1.28	1.22
6	A	350	HEM	CAB-C3B	2.01	1.52	1.47
6	A	350	HEM	C1A-CHA	-2.01	1.35	1.41

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	401	NAG	C2-N2-C7	13.62	141.15	122.90
9	A	411	NAG	C1-O5-C5	5.97	120.18	112.19
9	B	511	NAG	O5-C1-C2	5.12	114.67	109.52
10	A	501	BMA	O2-C2-C3	4.44	120.85	110.38
9	B	511	NAG	C3-C2-N2	-4.38	102.55	110.62
9	A	401	NAG	O5-C1-C2	-4.36	104.55	111.29
10	A	501	BMA	O5-C1-C2	3.84	117.06	110.30
6	A	350	HEM	C3B-C4B-NB	-3.56	106.91	109.47
9	B	511	NAG	C4-C3-C2	3.51	115.51	110.40
10	B	501	BMA	C3-C4-C5	3.49	116.56	110.23
6	A	350	HEM	C2C-C3C-C4C	3.36	109.24	106.90
6	A	350	HEM	C4B-C3B-C2B	3.25	110.27	107.28
9	A	401	NAG	C1-C2-N2	3.00	115.15	110.43
9	A	411	NAG	C4-C3-C2	-2.93	106.72	111.02
6	B	350	HEM	C4D-ND-C1D	2.91	108.66	105.21
10	A	501	BMA	O2-C2-C1	2.90	115.95	109.25
6	B	350	HEM	CHA-C4D-ND	2.89	127.96	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	350	HEM	C3B-C4B-NB	-2.88	107.40	109.47
9	B	511	NAG	O3-C3-C4	2.87	117.14	110.38
10	A	501	BMA	C1-C2-C3	2.64	115.74	110.36
9	A	411	NAG	O3-C3-C4	2.64	116.59	110.38
10	A	501	BMA	O3-C3-C2	2.63	116.58	110.38
6	A	350	HEM	CAA-CBA-CGA	-2.62	106.77	113.83
6	A	350	HEM	CBB-CAB-C3B	-2.59	114.59	127.53
9	B	511	NAG	O5-C5-C6	2.55	112.76	106.44
6	A	350	HEM	O2A-CGA-CBA	2.49	121.85	114.00
9	A	411	NAG	O3-C3-C2	-2.48	104.26	109.40
9	A	411	NAG	O5-C5-C4	2.47	116.83	110.83
6	A	350	HEM	O1A-CGA-CBA	-2.47	115.27	123.09
10	B	501	BMA	C4-C3-C2	2.42	115.08	110.83
9	A	401	NAG	O7-C7-C8	-2.42	117.75	122.05
9	B	511	NAG	C1-C2-C3	2.41	113.83	110.54
9	B	511	NAG	C6-C5-C4	2.37	118.83	113.02
6	A	350	HEM	CAD-C3D-C4D	2.36	128.81	124.70
6	B	350	HEM	C4B-C3B-C2B	2.33	109.42	107.28
6	A	350	HEM	CHA-C4D-ND	2.25	127.16	124.37
6	A	350	HEM	C4D-ND-C1D	2.23	107.85	105.21
6	A	350	HEM	CAD-CBD-CGD	-2.21	107.81	113.67
6	B	350	HEM	CMA-C3A-C4A	-2.14	125.33	128.46
6	B	350	HEM	CAA-CBA-CGA	-2.13	108.10	113.83
6	B	350	HEM	CBA-CAA-C2A	-2.12	108.98	112.54
6	A	350	HEM	C1D-C2D-C3D	-2.09	104.79	106.98
9	B	511	NAG	C2-N2-C7	2.08	127.98	123.11
6	B	350	HEM	O1A-CGA-CBA	-2.03	116.66	123.09
6	A	350	HEM	CMD-C2D-C1D	2.03	128.20	125.03

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	401	NAG	C8-C7-N2-C2
9	A	401	NAG	O7-C7-N2-C2
13	B	1355	TRS	C2-C-C1-O1
13	B	1355	TRS	C1-C-C2-O2
13	B	1355	TRS	C3-C-C2-O2
13	B	1355	TRS	N-C-C2-O2
13	B	1355	TRS	C1-C-C3-O3
13	B	1355	TRS	C2-C-C3-O3
13	B	1355	TRS	N-C-C3-O3

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Mol	Chain	Res	Type	Atoms
10	A	501	BMA	O5-C5-C6-O6
9	B	411	NAG	C4-C5-C6-O6
10	B	501	BMA	O5-C5-C6-O6
10	A	501	BMA	C4-C5-C6-O6
9	A	401	NAG	O5-C5-C6-O6
9	B	411	NAG	O5-C5-C6-O6
10	B	501	BMA	C4-C5-C6-O6
9	A	401	NAG	C4-C5-C6-O6
9	A	411	NAG	C8-C7-N2-C2
9	A	411	NAG	O7-C7-N2-C2
9	A	391	NAG	O5-C5-C6-O6
9	A	391	NAG	C4-C5-C6-O6
13	B	1355	TRS	C3-C-C1-O1
13	B	1355	TRS	N-C-C1-O1
6	B	350	HEM	CAA-CBA-CGA-O2A
6	A	350	HEM	CAA-CBA-CGA-O1A
6	B	350	HEM	CAA-CBA-CGA-O1A
6	A	350	HEM	CAA-CBA-CGA-O2A

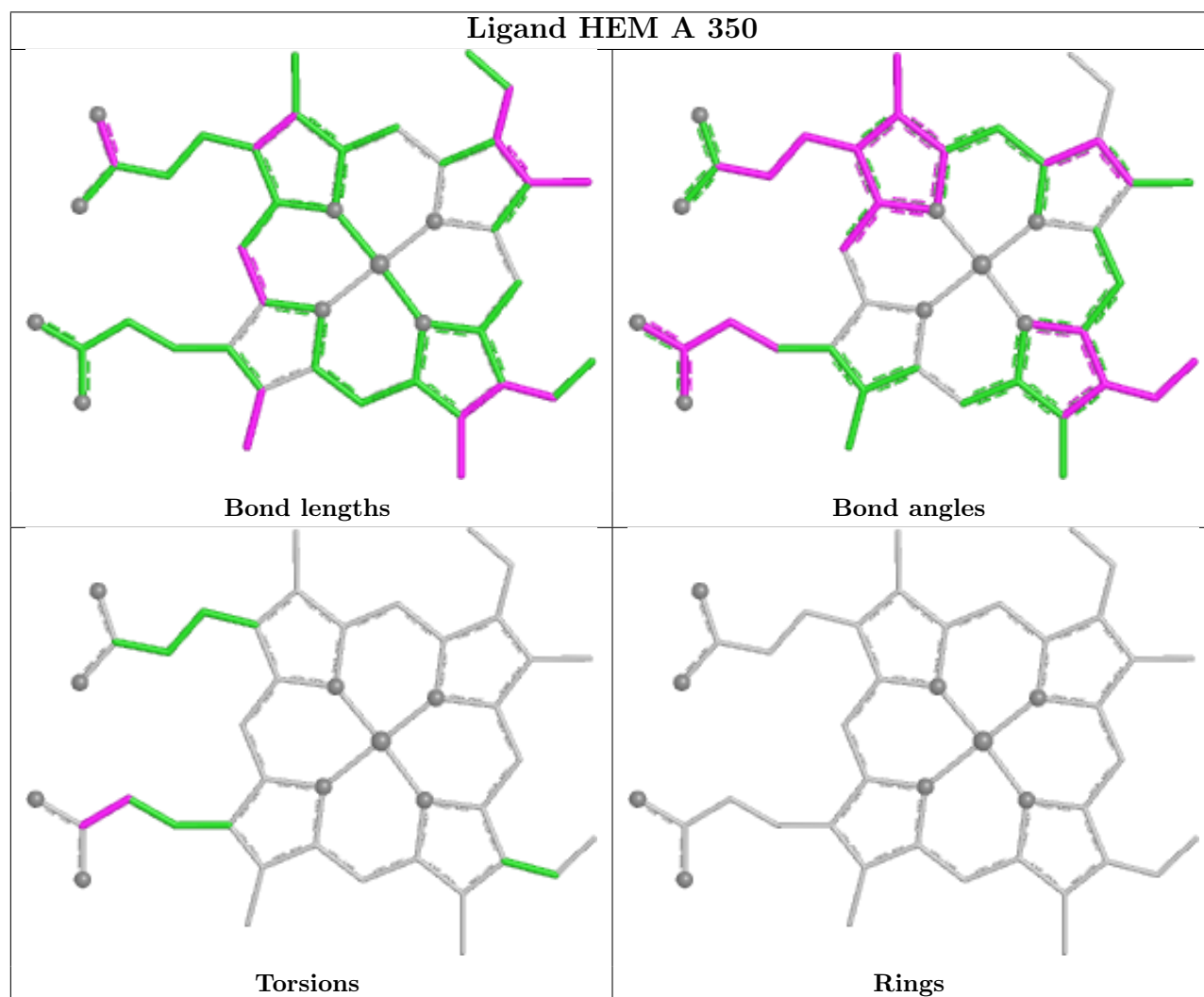
There are no ring outliers.

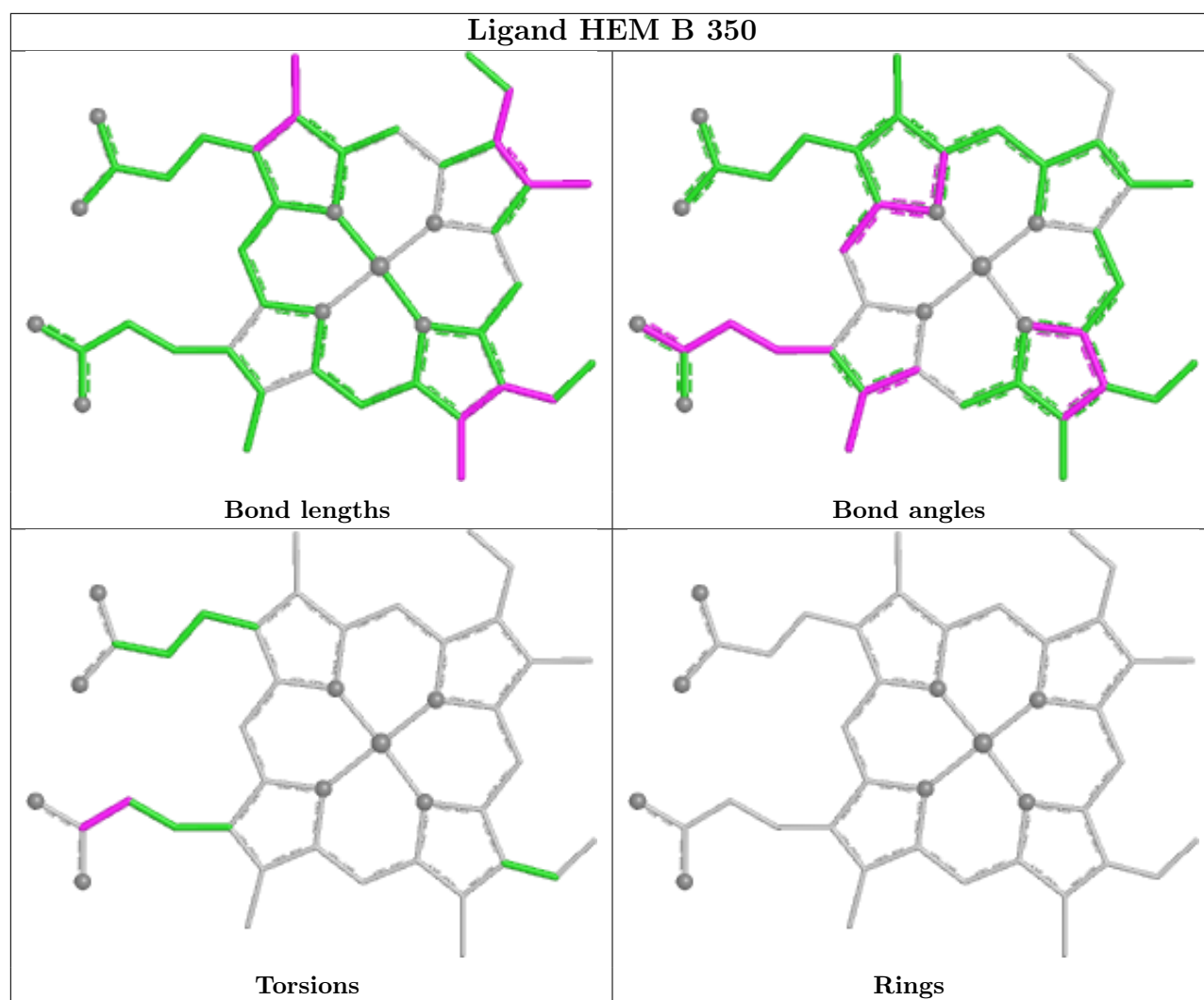
8 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	1355	TRS	1	0
9	B	511	NAG	4	0
11	B	1357	SO4	1	0
6	A	350	HEM	4	0
6	B	350	HEM	2	0
9	A	401	NAG	6	0
10	A	501	BMA	3	0
10	B	501	BMA	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	324/325 (99%)	-0.38	3 (0%) 84 83	8, 18, 32, 77	0
1	B	324/325 (99%)	-0.35	3 (0%) 84 83	6, 16, 31, 68	0
All	All	648/650 (99%)	-0.36	6 (0%) 84 83	6, 17, 32, 77	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	327	ARG	5.6
1	B	326	GLY	3.6
1	A	328	ASP	3.5
1	A	327	ARG	3.0
1	A	326	GLY	2.7
1	B	10	GLU	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	NAG	J	2	14/15	0.14	0.67	95,96,97,97	0
3	MAN	D	5	11/12	0.46	0.28	80,82,84,84	0
5	NAG	J	1	14/15	0.48	0.60	77,83,86,91	0

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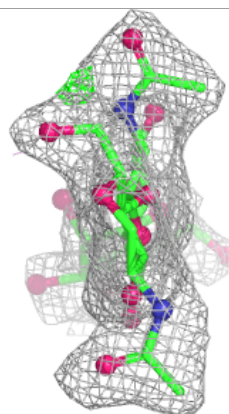
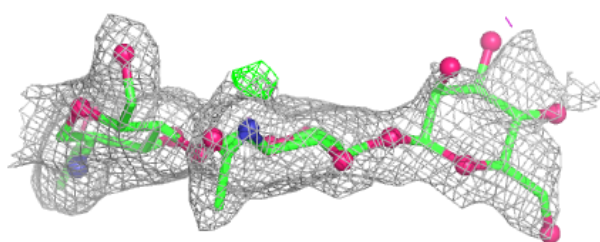
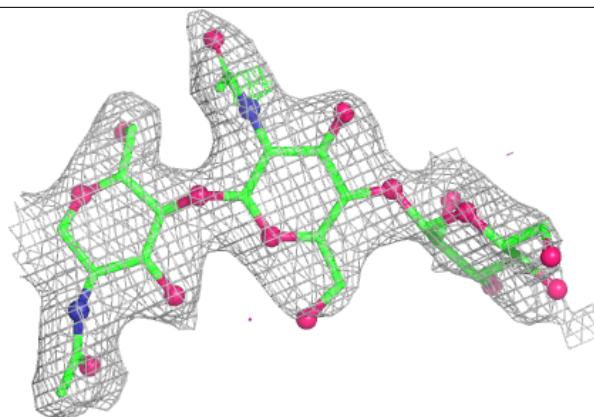
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BMA	E	3	11/12	0.50	0.56	89,90,92,93	0
4	MAN	F	6	11/12	0.52	0.62	67,71,72,73	0
3	MAN	D	4	11/12	0.65	0.34	89,92,93,95	0
5	NAG	H	2	14/15	0.69	0.42	72,75,76,77	0
5	NAG	I	2	14/15	0.70	0.44	68,73,76,77	0
2	NAG	E	2	14/15	0.71	0.33	72,76,79,84	0
3	BMA	D	3	11/12	0.73	0.27	74,78,83,84	0
5	NAG	G	2	14/15	0.77	0.21	44,52,57,60	0
4	MAN	F	7	11/12	0.79	0.32	53,57,60,63	0
2	BMA	C	3	11/12	0.79	0.42	70,72,74,74	0
5	NAG	I	1	14/15	0.85	0.28	41,46,50,61	0
5	NAG	H	1	14/15	0.87	0.20	41,51,58,65	0
3	NAG	D	2	14/15	0.87	0.21	46,51,58,66	0
2	NAG	C	2	14/15	0.88	0.21	43,51,59,64	0
2	NAG	E	1	14/15	0.89	0.25	39,50,57,65	0
4	MAN	F	5	11/12	0.90	0.24	46,48,52,59	0
4	MAN	F	8	11/12	0.91	0.19	38,42,43,43	0
4	MAN	F	4	11/12	0.91	0.19	40,44,47,50	0
4	BMA	F	3	11/12	0.92	0.23	39,42,44,46	0
4	NAG	F	1	14/15	0.93	0.10	21,24,27,28	0
4	NAG	F	2	14/15	0.94	0.15	30,32,38,39	0
2	NAG	C	1	14/15	0.94	0.13	30,35,41,48	0
5	NAG	G	1	14/15	0.95	0.09	9,12,24,32	0
3	NAG	D	1	14/15	0.96	0.09	10,21,30,35	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.

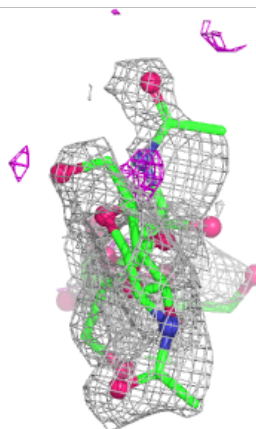
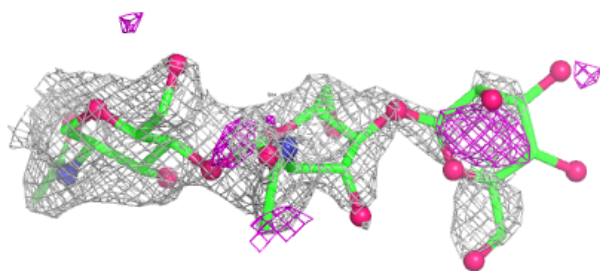
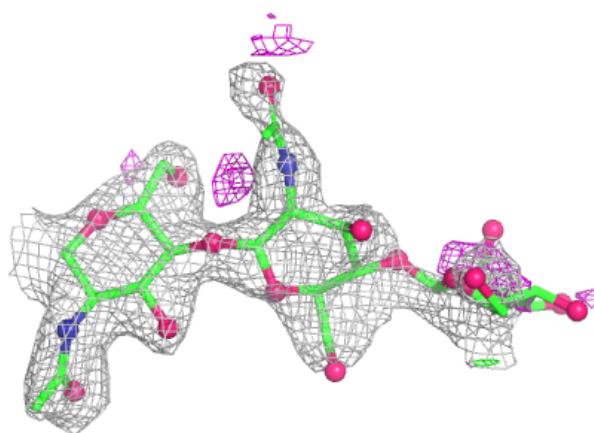


**Electron density around Chain C:**

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

**Electron density around Chain E:**

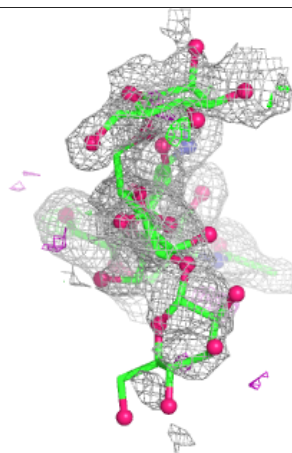
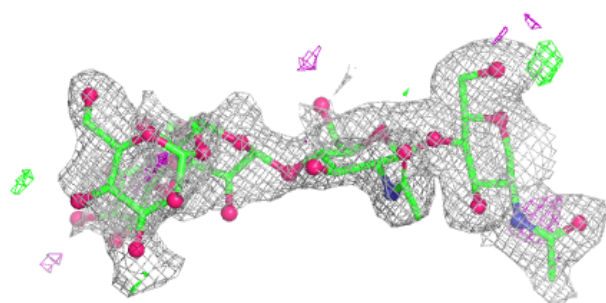
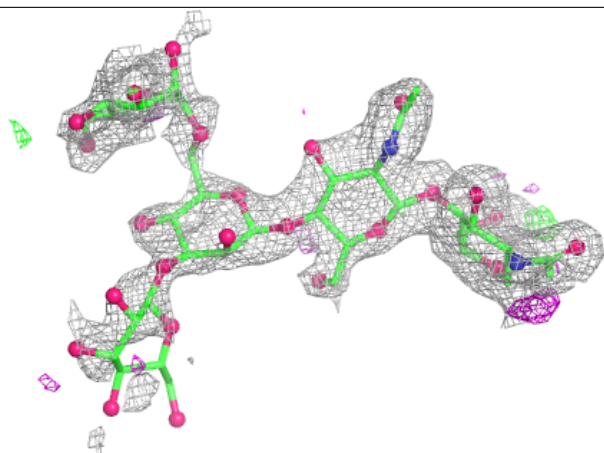
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





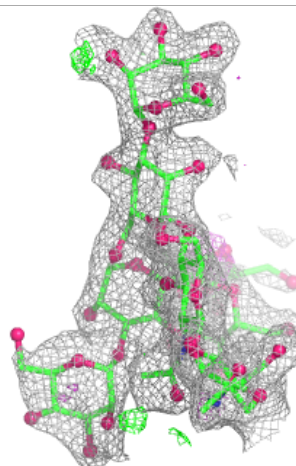
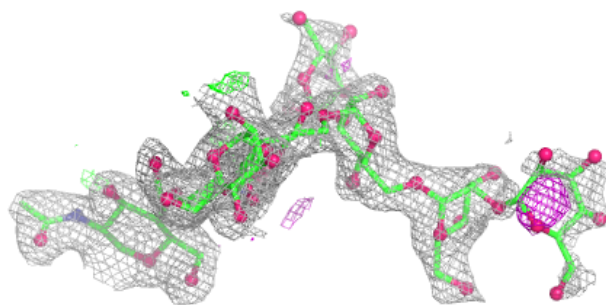
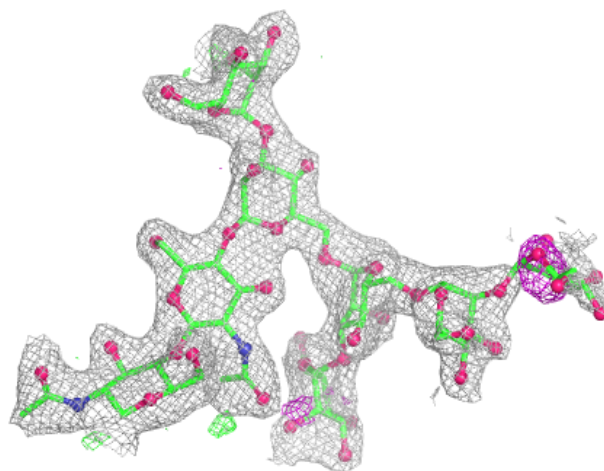
**Electron density around Chain D:**

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



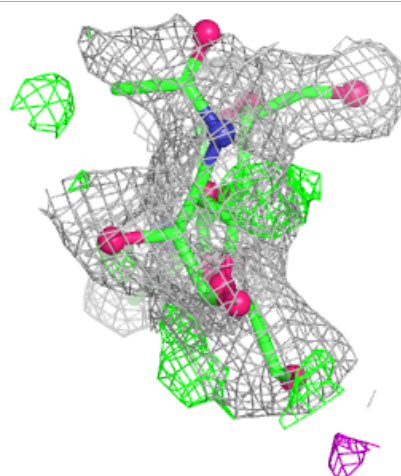
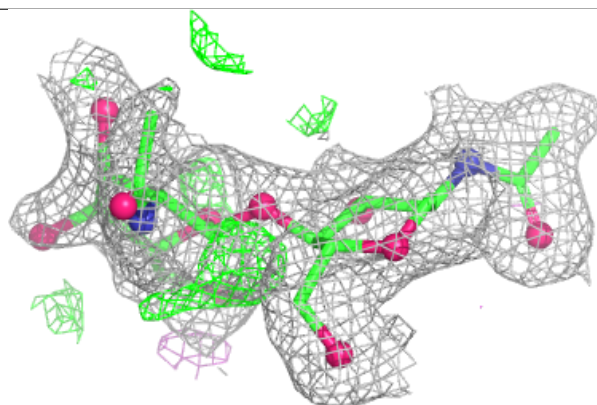
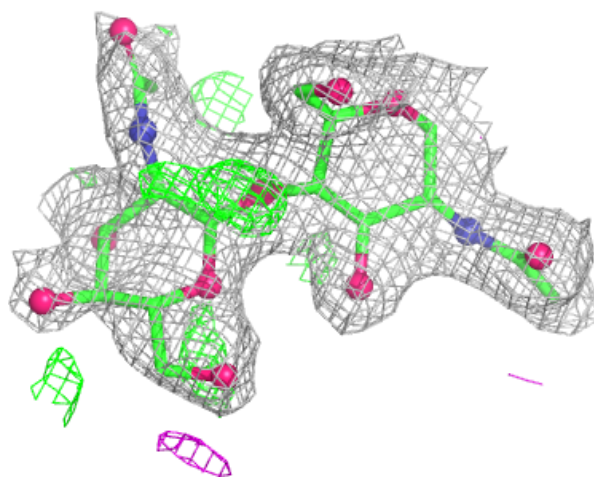
**Electron density around Chain F:**

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



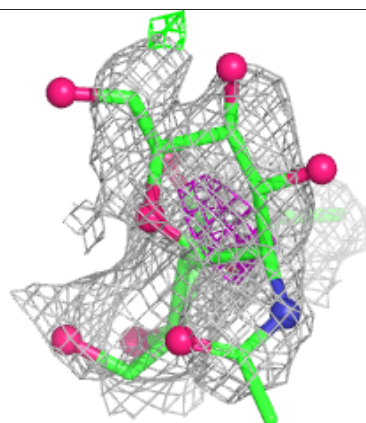
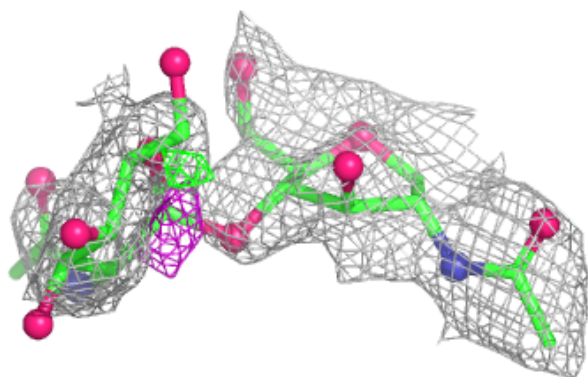
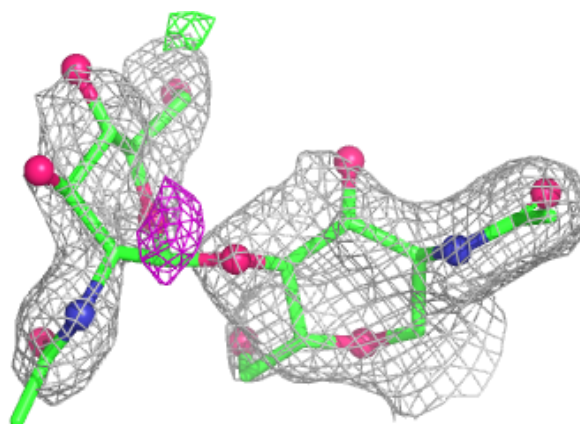
**Electron density around Chain G:**

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



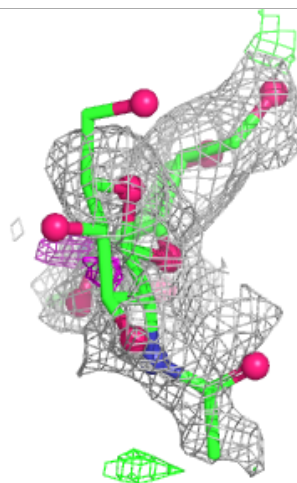
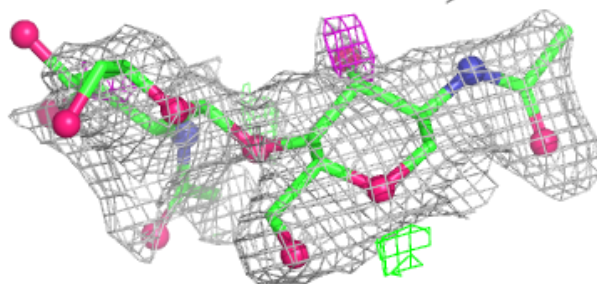
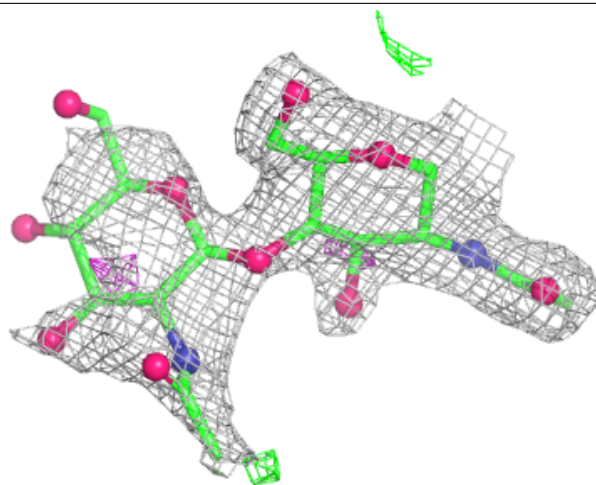
**Electron density around Chain H:**

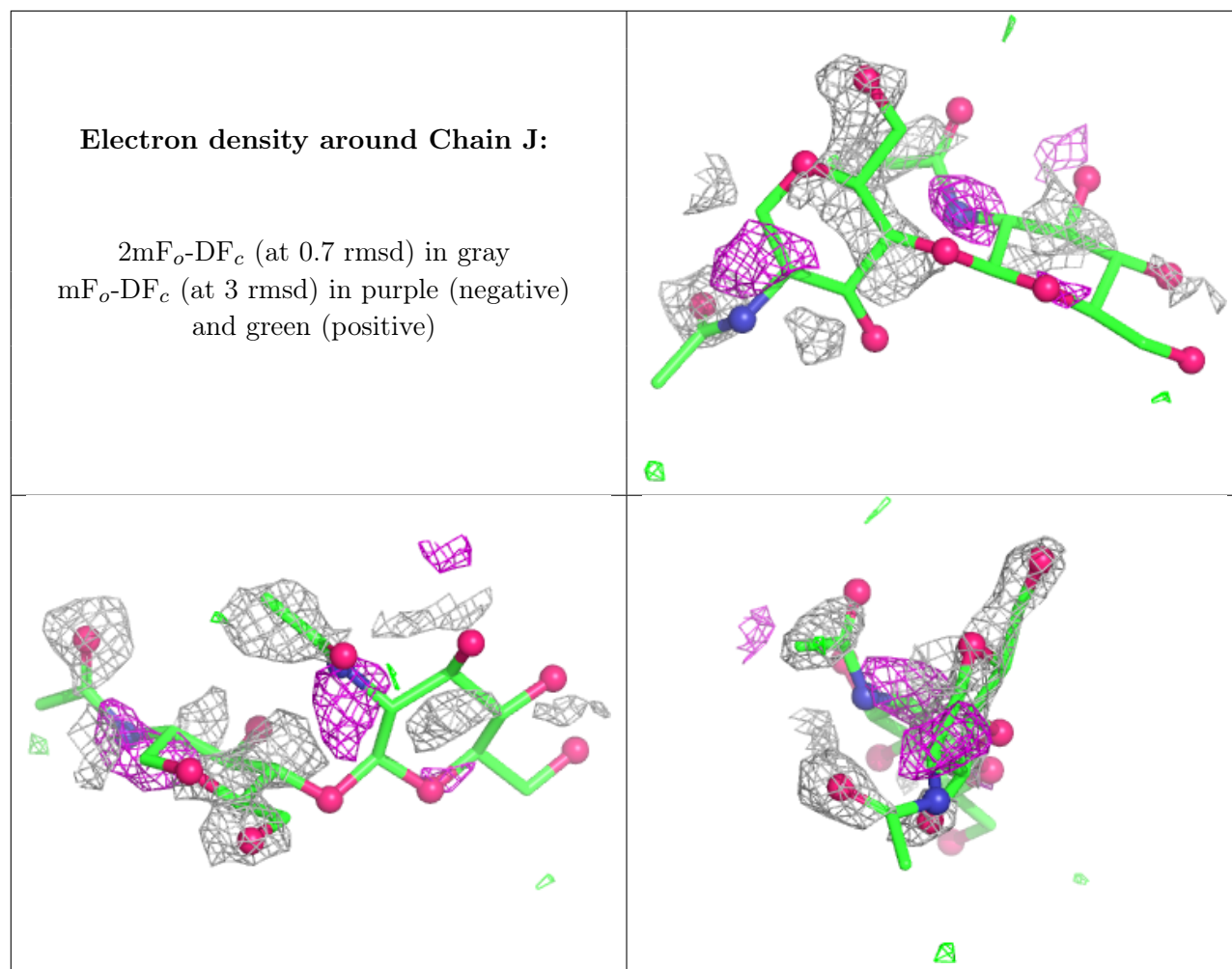
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
13	TRS	B	1355	8/8	0.58	0.47	88,89,90,90	0
9	NAG	B	411	14/15	0.62	0.66	71,77,81,81	0
10	BMA	B	501	12/12	0.66	0.36	48,55,57,57	0
9	NAG	A	401	14/15	0.68	0.47	66,70,72,73	0
9	NAG	A	391	14/15	0.70	0.28	39,54,65,66	0
9	NAG	B	511	15/15	0.71	0.40	48,54,60,61	0
9	NAG	A	411	14/15	0.80	0.37	57,61,66,68	0
10	BMA	A	501	12/12	0.83	0.37	22,37,43,45	0
12	CL	B	1358	1/1	0.91	0.05	68,68,68,68	0
11	SO4	B	1360	5/5	0.92	0.13	48,50,54,55	0

*Continued on next page...*



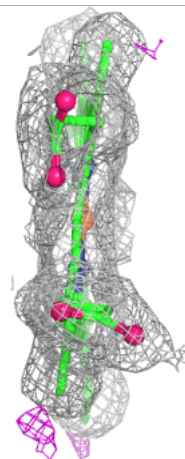
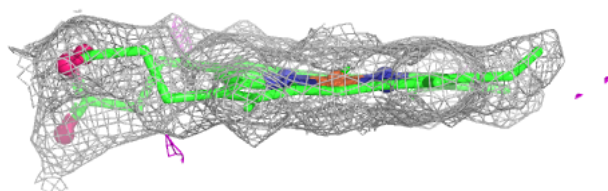
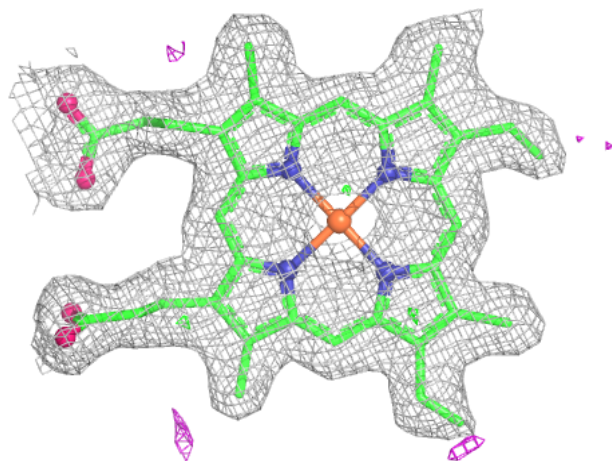
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
11	SO4	B	1359	5/5	0.94	0.27	68,68,70,72	0
11	SO4	A	1355	5/5	0.94	0.24	81,81,82,82	0
12	CL	B	1361	1/1	0.95	0.06	51,51,51,51	0
11	SO4	A	1358	5/5	0.96	0.14	75,76,77,77	0
8	MZ0	A	354	7/7	0.96	0.12	15,17,23,27	0
8	MZ0	B	354	7/7	0.96	0.15	15,18,26,33	0
11	SO4	B	1357	5/5	0.97	0.08	44,45,46,48	0
6	HEM	B	350	43/43	0.98	0.12	2,7,14,16	0
12	CL	B	1356	1/1	0.98	0.05	34,34,34,34	0
7	MG	A	353	1/1	0.98	0.09	8,8,8,8	0
7	MG	B	353	1/1	0.98	0.07	9,9,9,9	0
6	HEM	A	350	43/43	0.98	0.10	6,8,16,20	0
11	SO4	A	1357	5/5	0.99	0.09	40,41,43,45	0
12	CL	A	1356	1/1	0.99	0.05	35,35,35,35	0

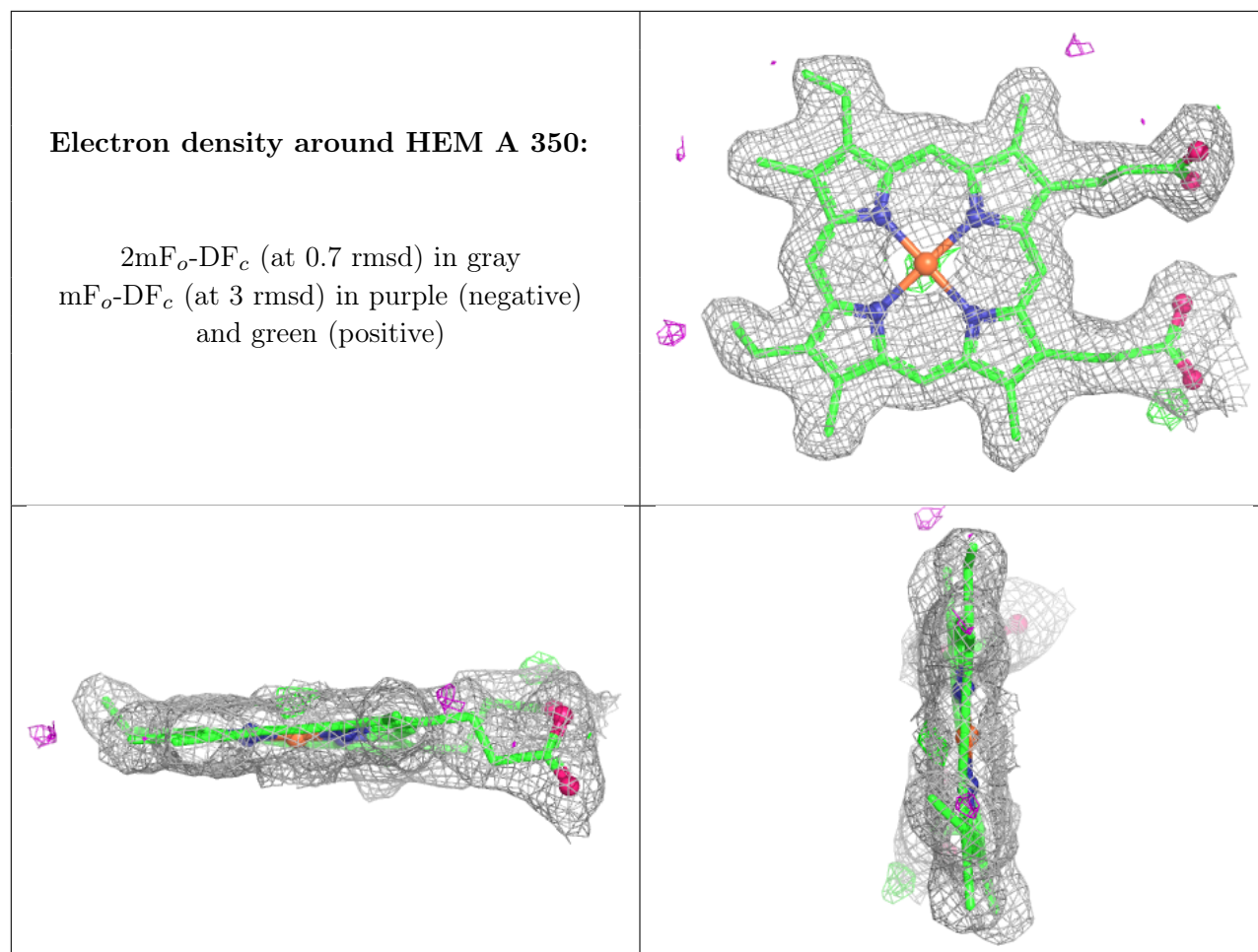
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around HEM B 350:**

$2mF_o-DF_c$  (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.