



wwPDB X-ray Structure Validation Summary 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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-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

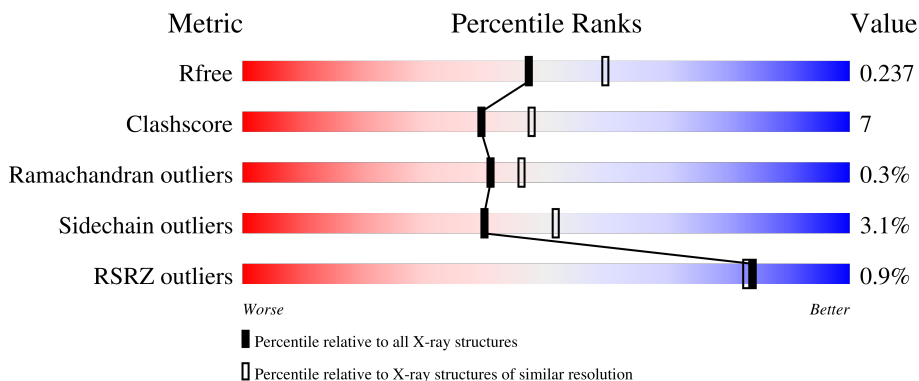
1 Overall quality at a glance i

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.



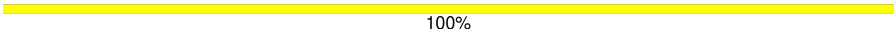
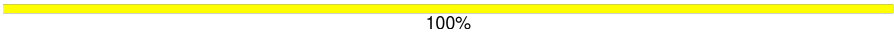

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 ≥ 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	
1	B	325	
2	C	3	
2	E	3	
3	D	5	

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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.

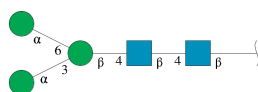
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	324	Total	C	N	O	S	0	0	0
			2513	1590	438	477	8			
1	B	324	Total	C	N	O	S	0	2	0
			2521	1598	438	477	8			

- 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
			Total	C	N	O			
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			

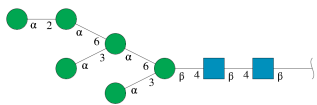
- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
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.



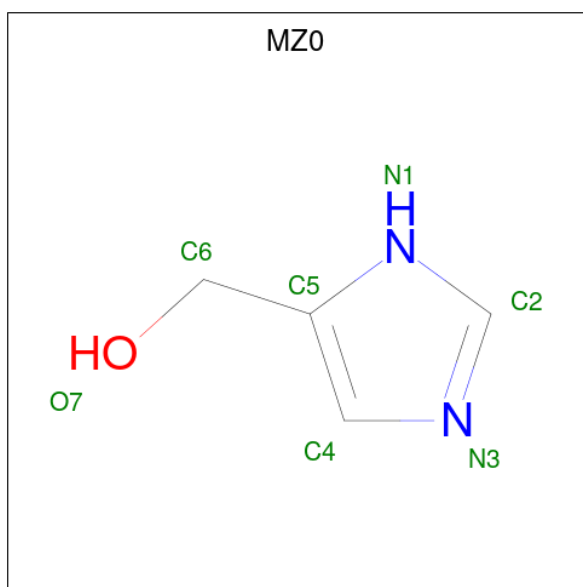
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	F	8	94	52	2	40	0	0	0

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

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



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: $C_8H_{15}NO_6$).



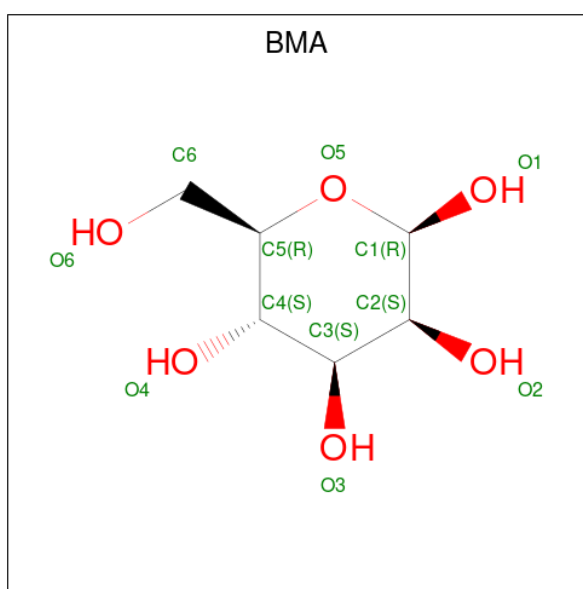
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		

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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: C₆H₁₂O₆).



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: O₄S).

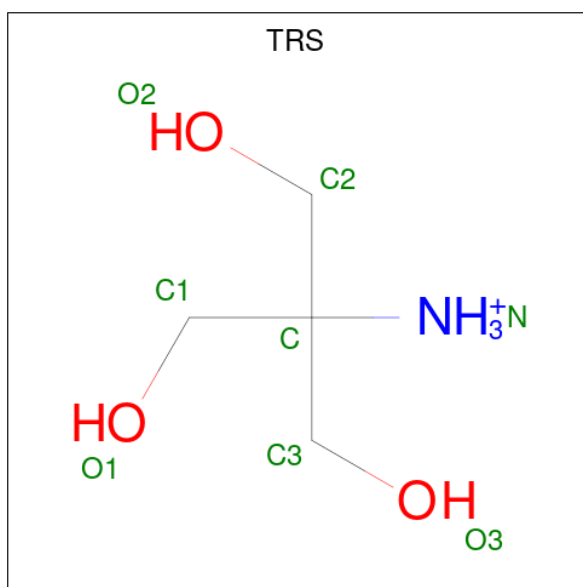


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total O S 5 4 1	0	0
11	A	1	Total O S 5 4 1	0	0
11	A	1	Total O S 5 4 1	0	0
11	B	1	Total O S 5 4 1	0	0
11	B	1	Total O S 5 4 1	0	0
11	B	1	Total O S 5 4 1	0	0

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

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

- Molecule 13 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



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

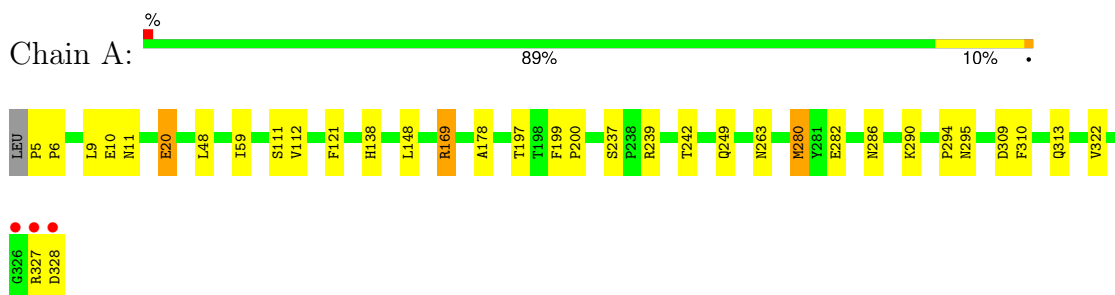
- Molecule 14 is water.

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

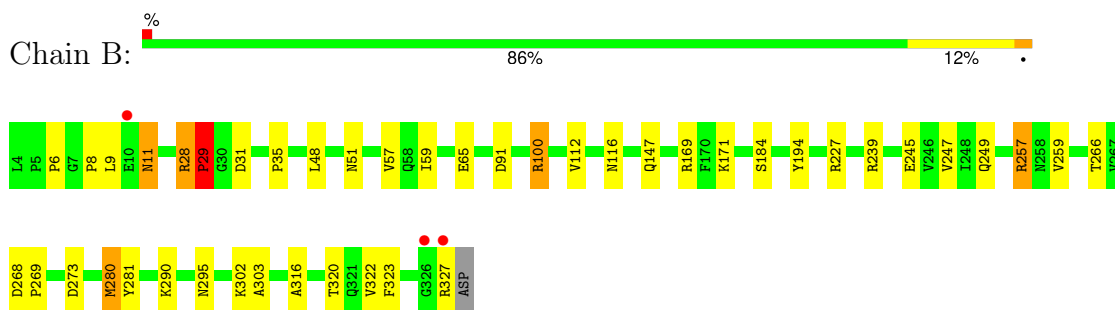
3 Residue-property plots [i](#)

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



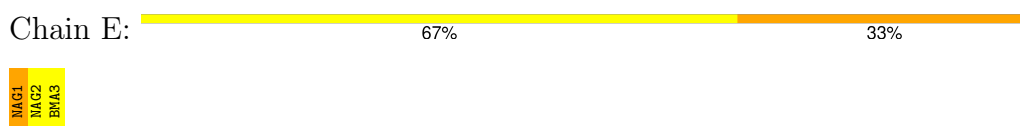
- Molecule 1: AROMATIC PEROXYGENASE



- 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%

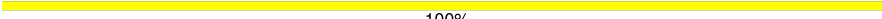

- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	4.46 (at 2.20Å)	Xtrriage
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 ²)	17.6	Xtrriage
Anisotropy	0.258	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6261	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage'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.*

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 [i](#)

5.1 Standard geometry [i](#)

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 [i](#)

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.

The worst 5 of 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

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	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 [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	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

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	290	LYS
1	B	327	ARG
1	A	290	LYS
1	B	28	ARG
1	B	100	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

The worst 5 of 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
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

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	J	1	NAG	C1

5 of 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

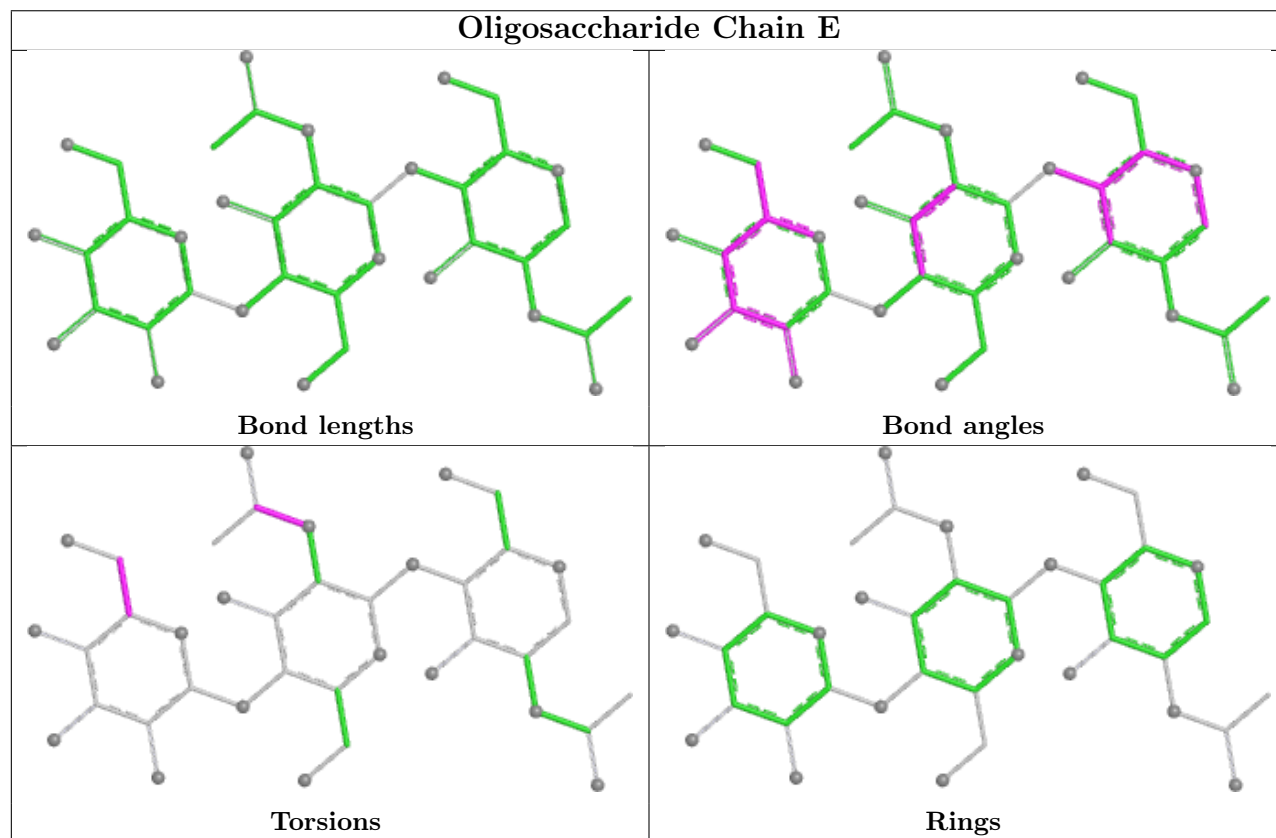
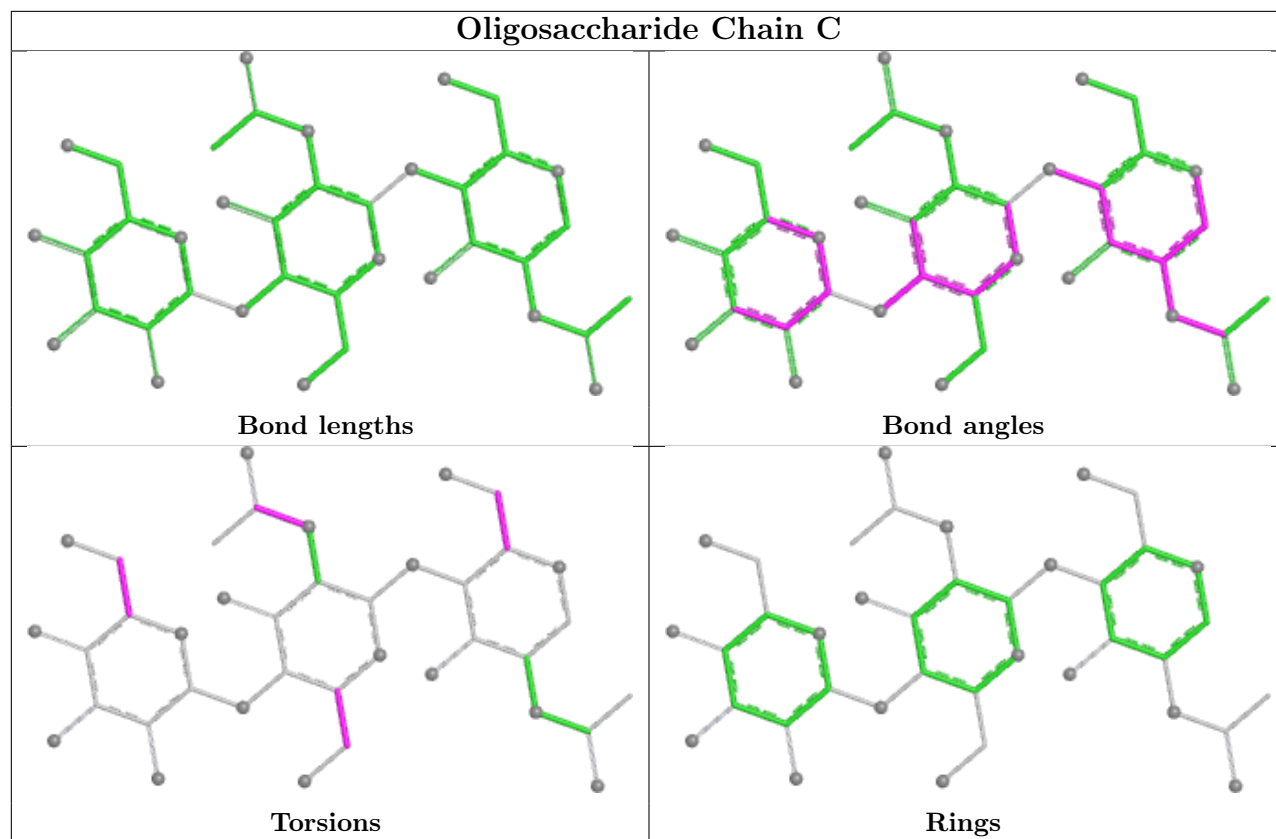
All (1) ring outliers are listed below:

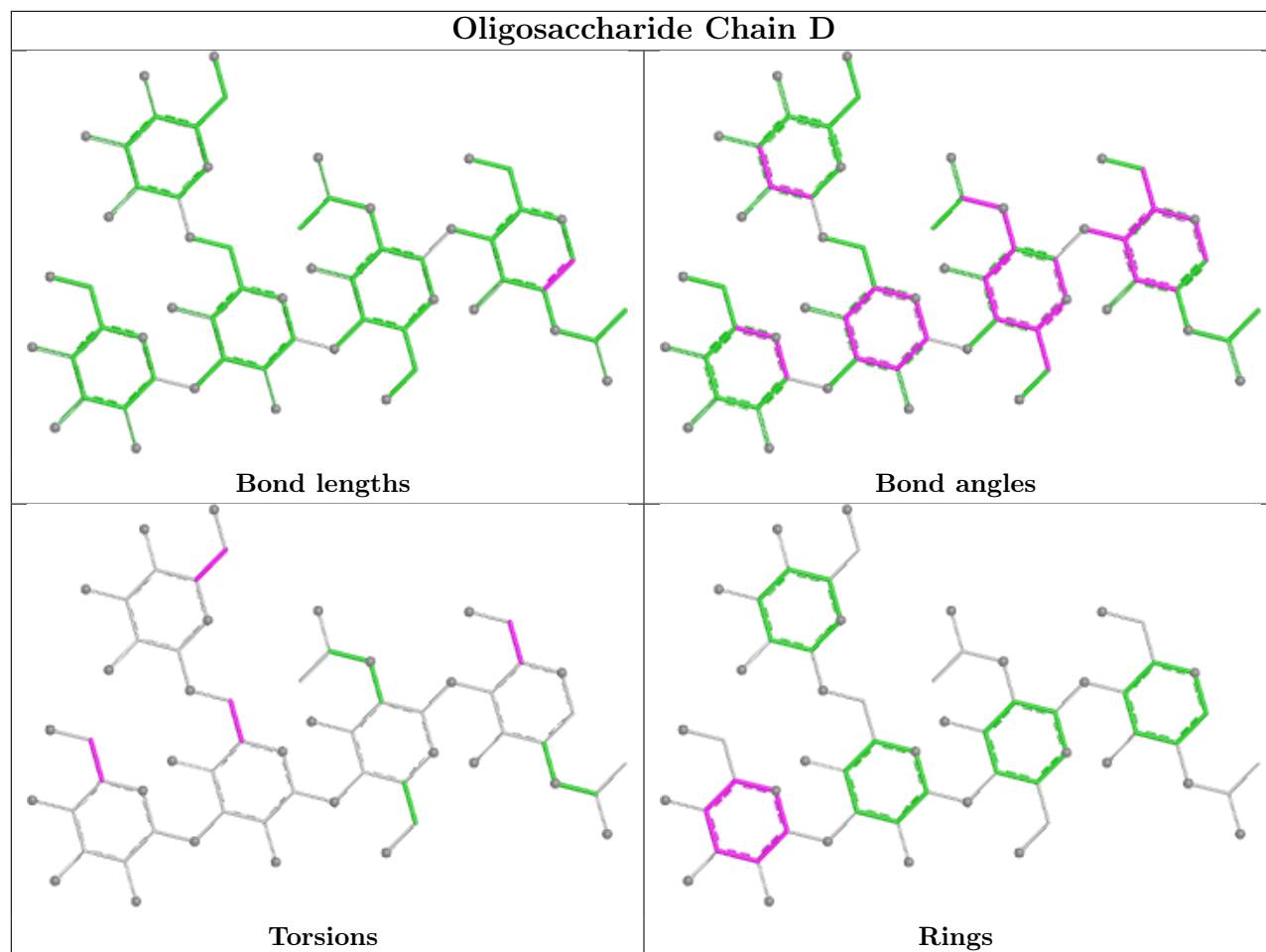
Mol	Chain	Res	Type	Atoms
3	D	4	MAN	C1-C2-C3-C4-C5-O5

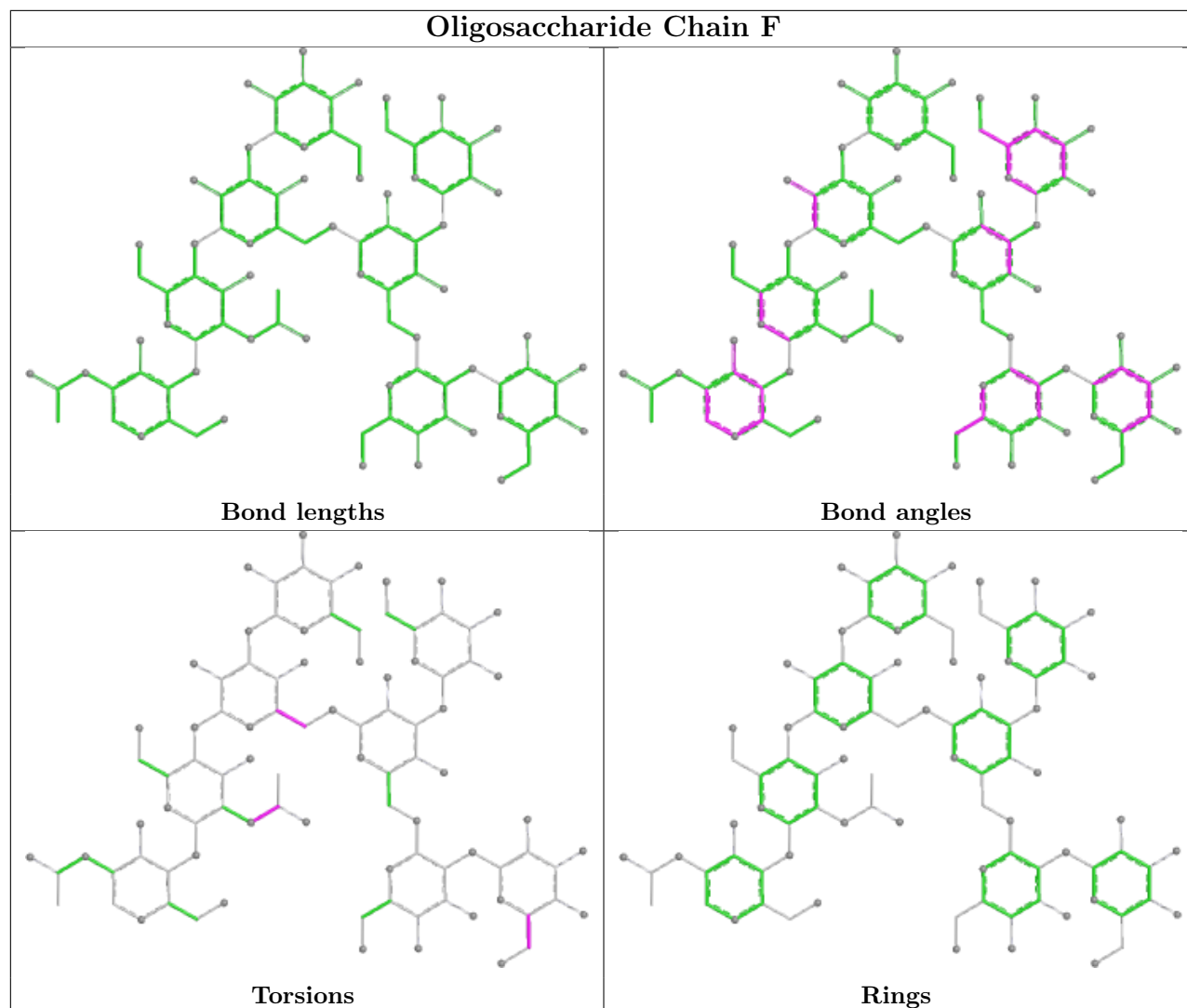
7 monomers are involved in 7 short contacts:

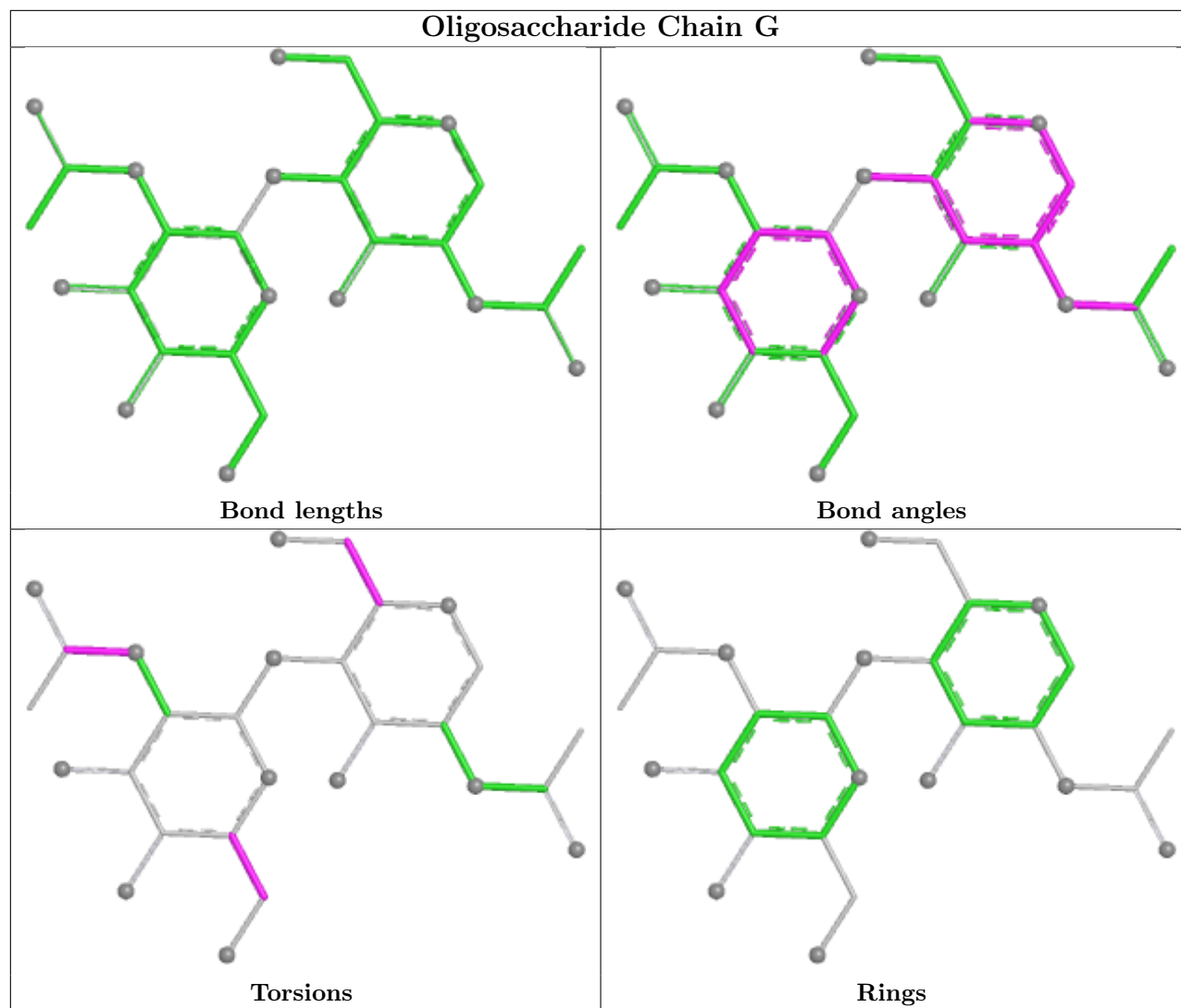
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0
5	J	1	NAG	2	0
2	C	3	BMA	2	0
2	C	2	NAG	2	0
3	D	5	MAN	2	0
5	J	2	NAG	2	0
3	D	3	BMA	2	0

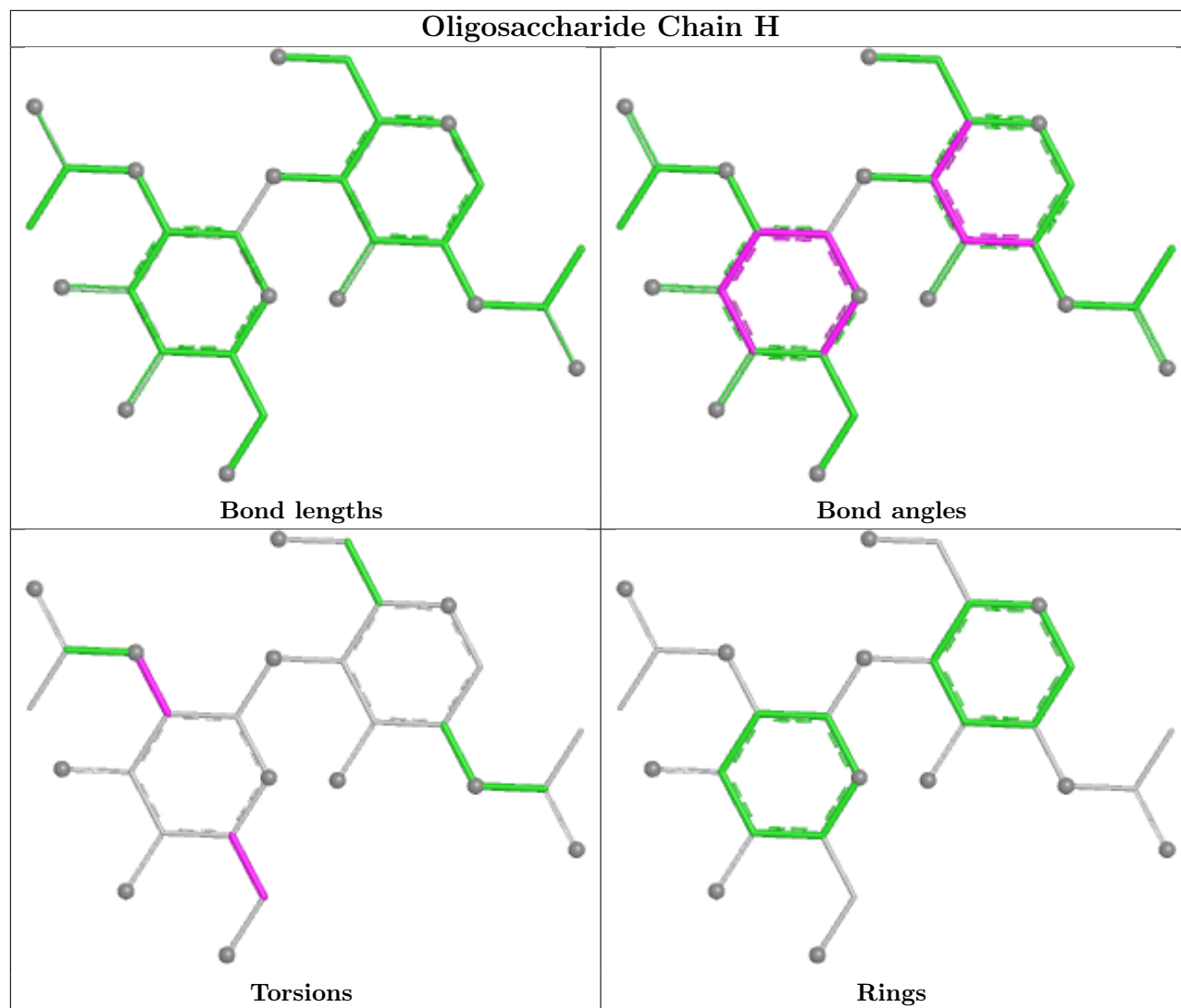
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

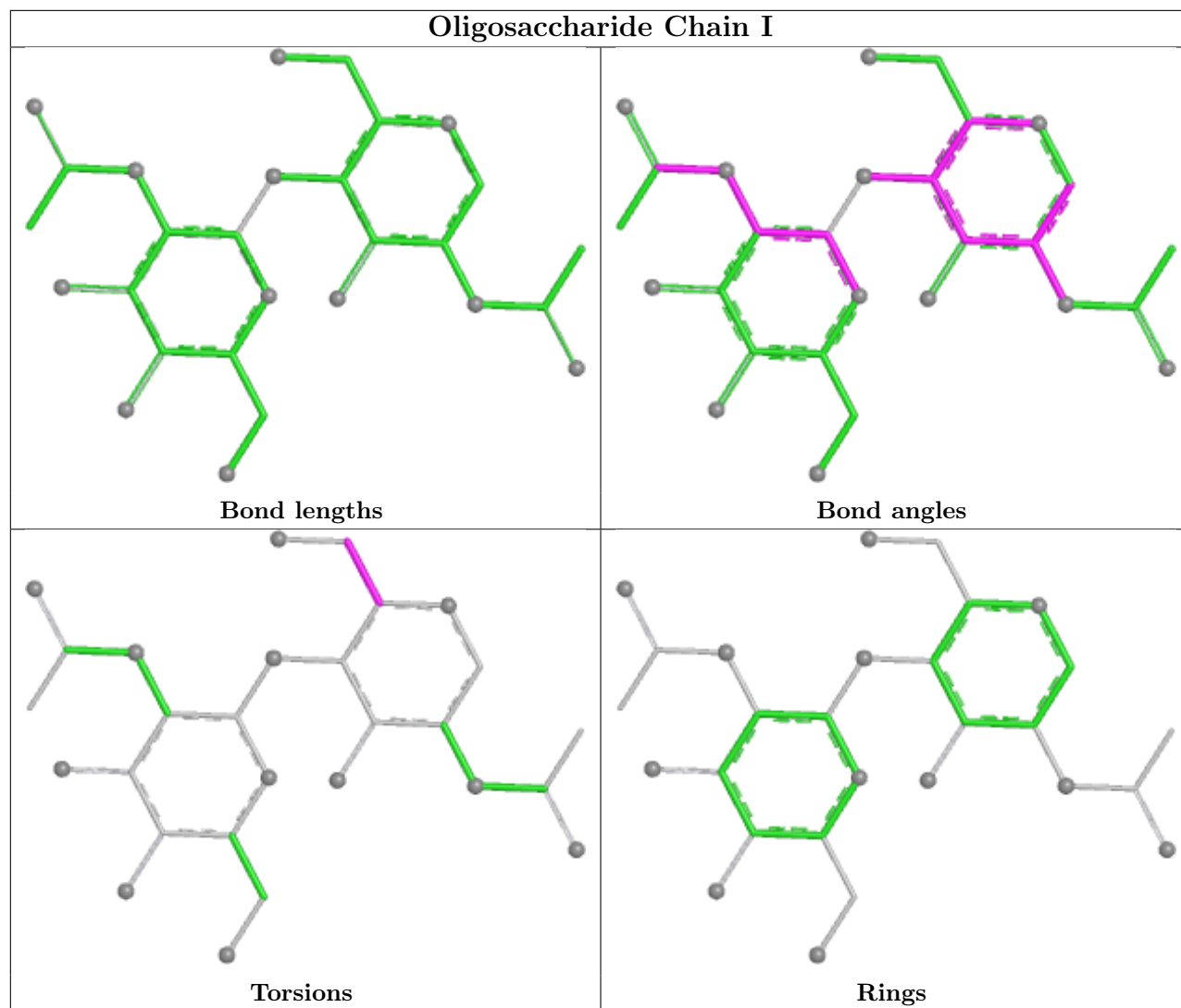


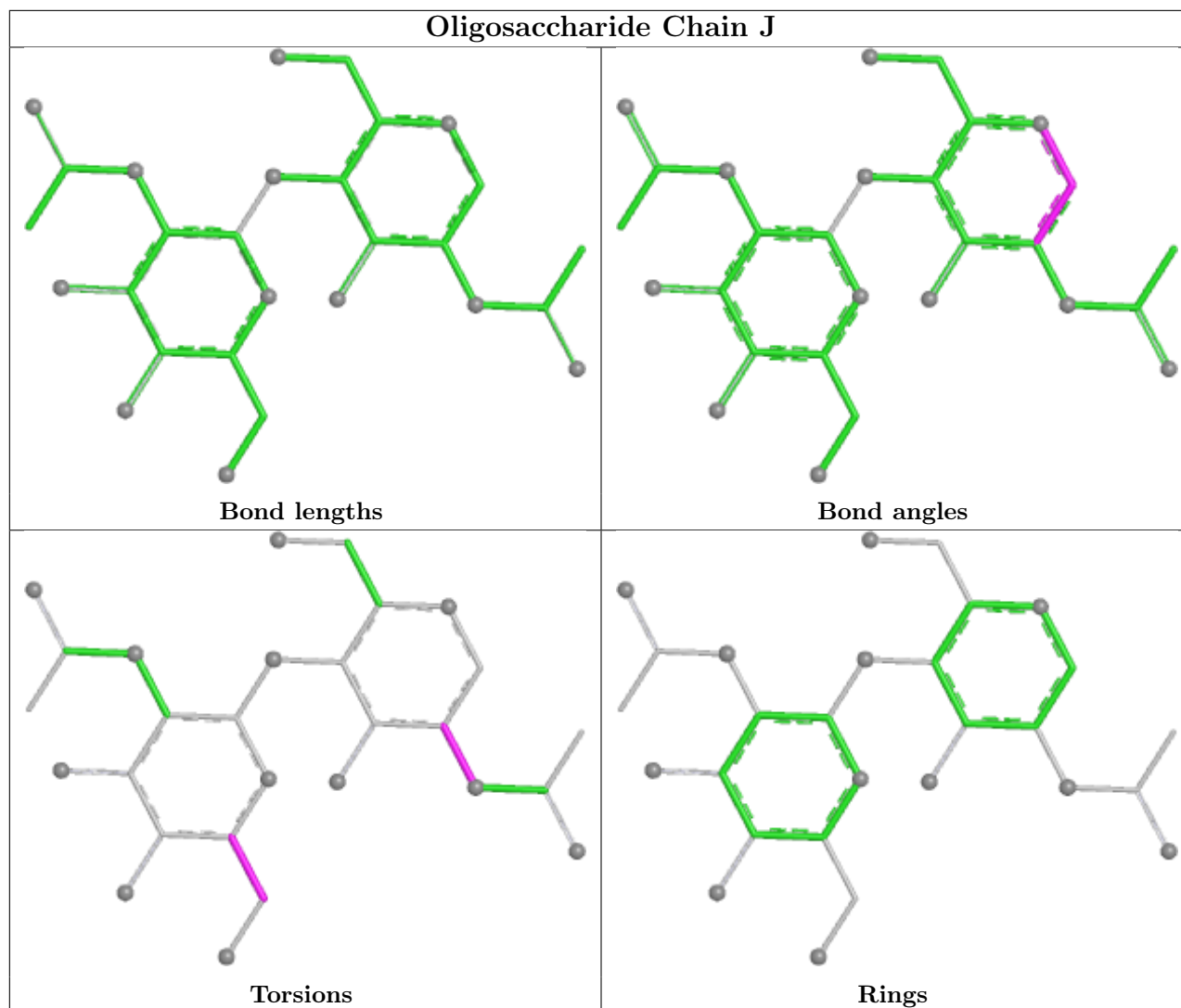












5.6 Ligand geometry [i](#)

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

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 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

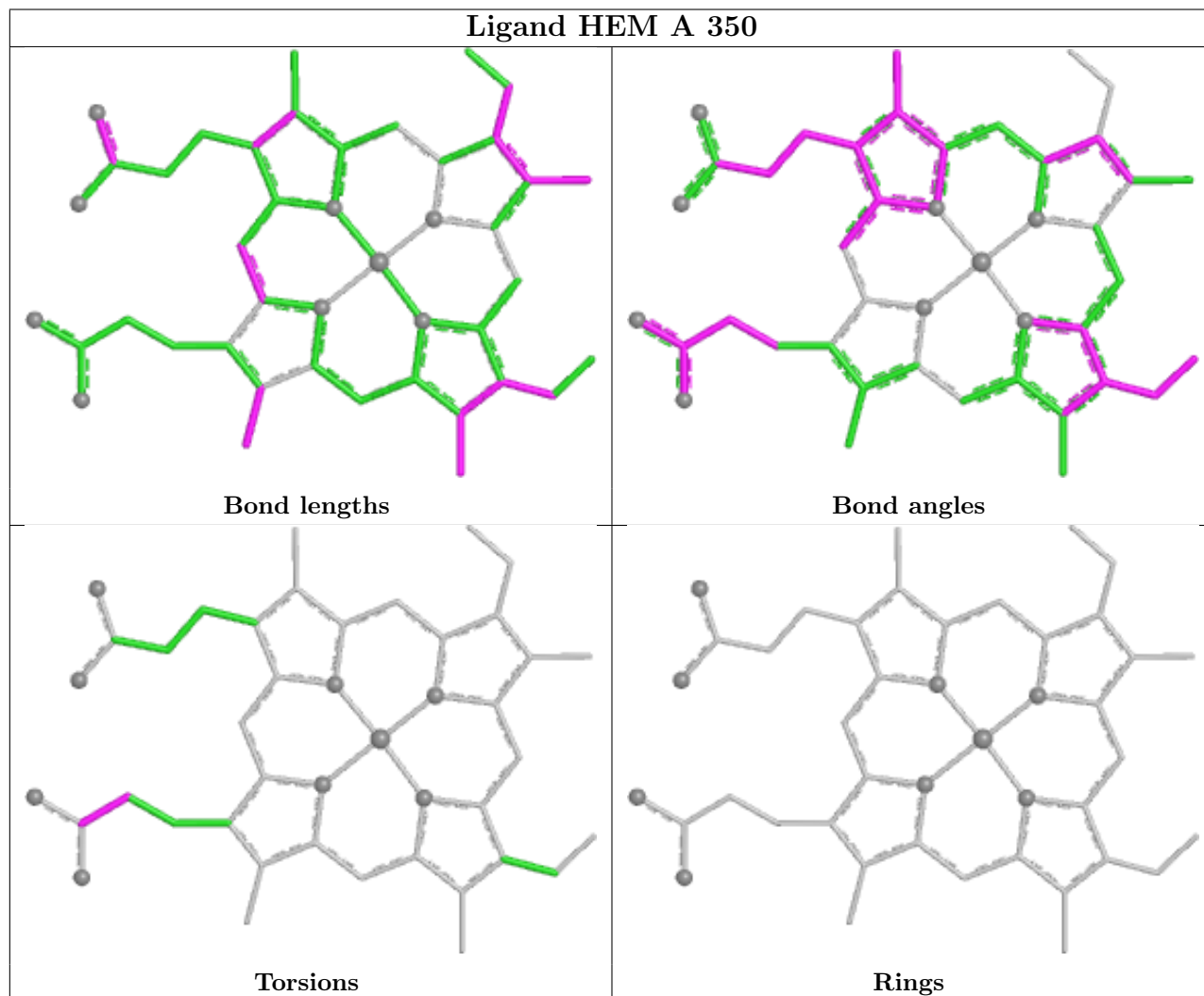
There are no ring outliers.

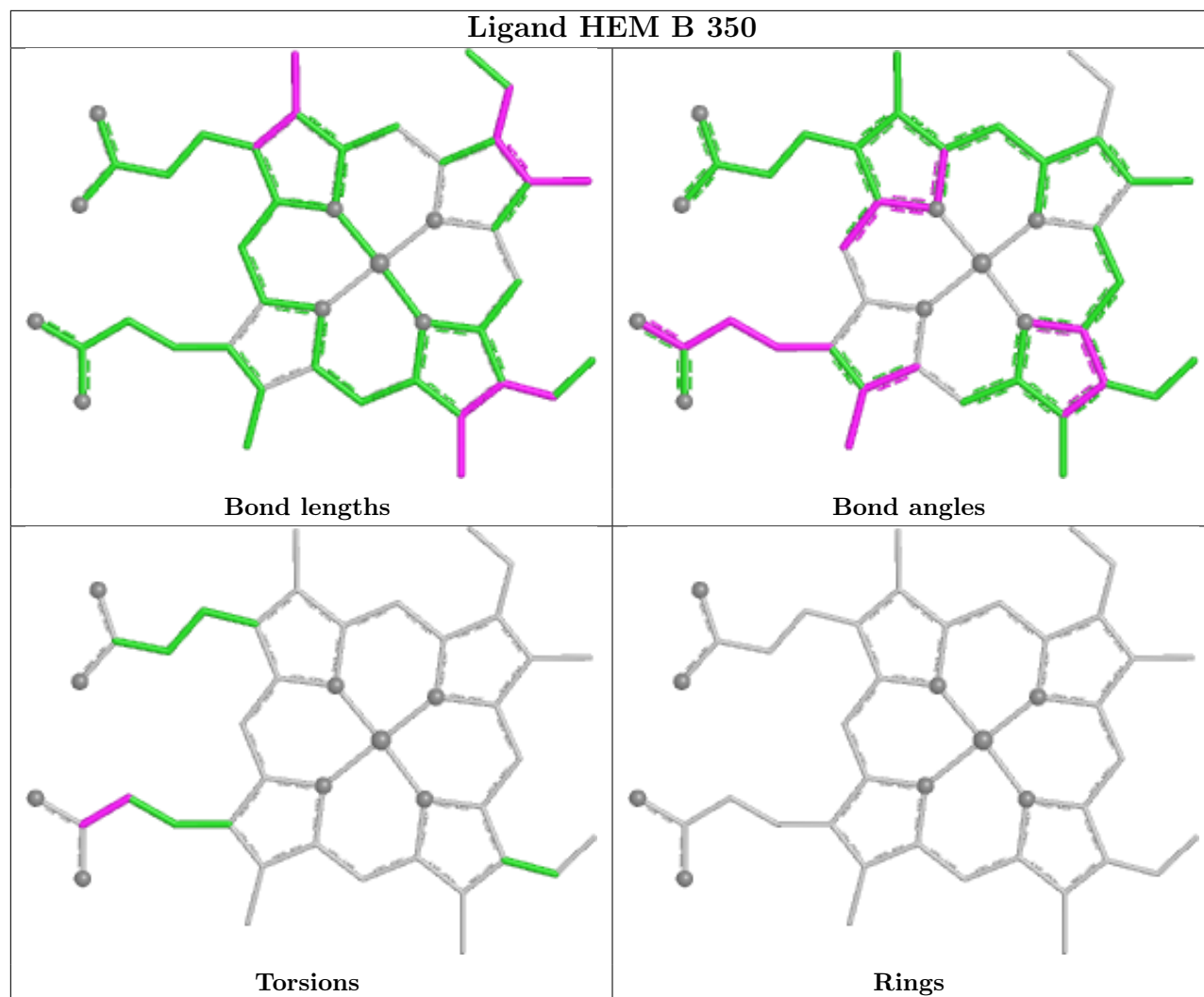
8 monomers are involved in 24 short contacts:

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	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

The worst 5 of 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

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
2	BMA	E	3	11/12	0.50	0.56	89,90,92,93	0

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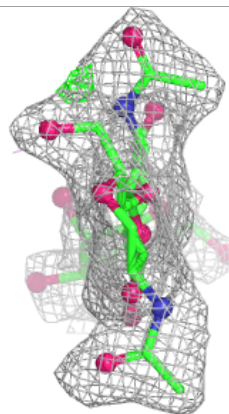
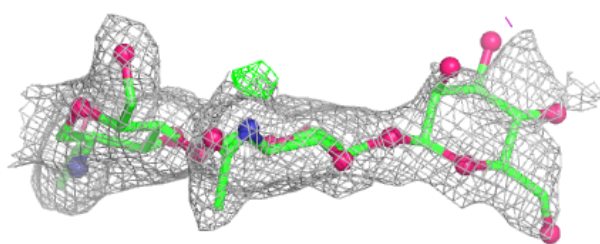
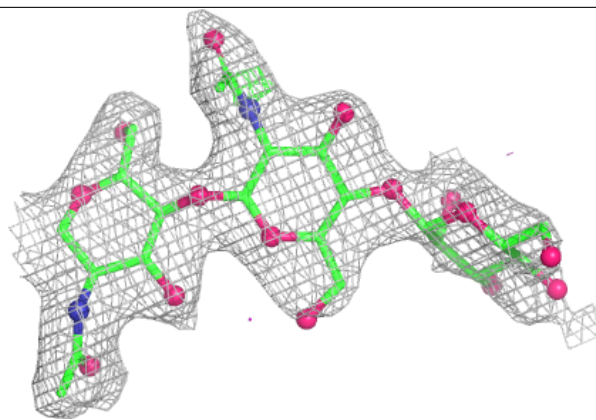
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MAN	F	6	11/12	0.52	0.62	67,71,72,73	0
3	MAN	D	4	11/12	0.65	0.34	89,92,93,95	0
5	NAG	H	2	14/15	0.69	0.42	72,75,76,77	0
5	NAG	I	2	14/15	0.70	0.44	68,73,76,77	0
2	NAG	E	2	14/15	0.71	0.33	72,76,79,84	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

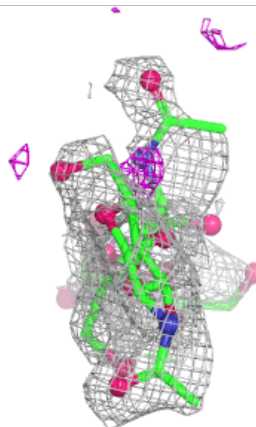
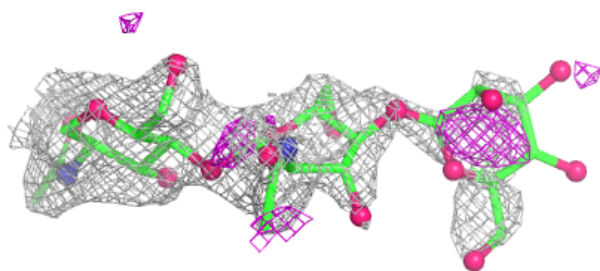
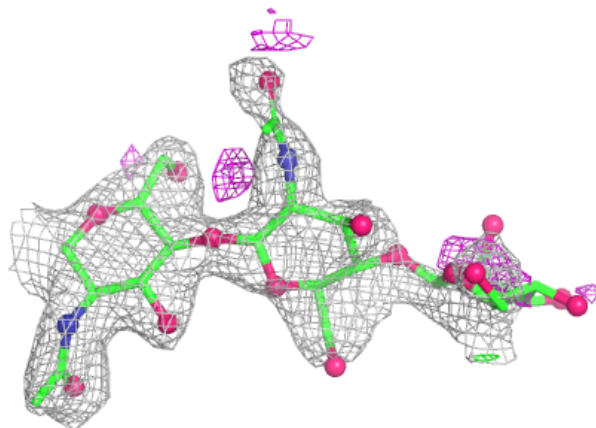
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

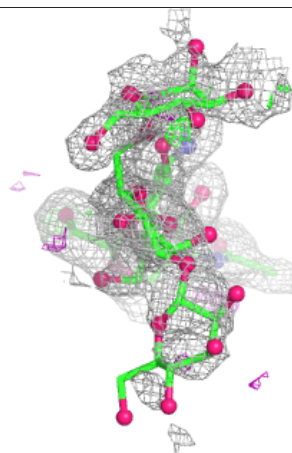
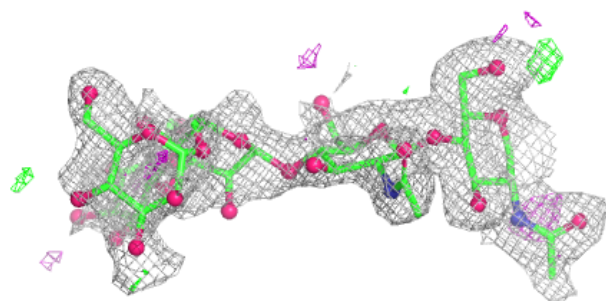
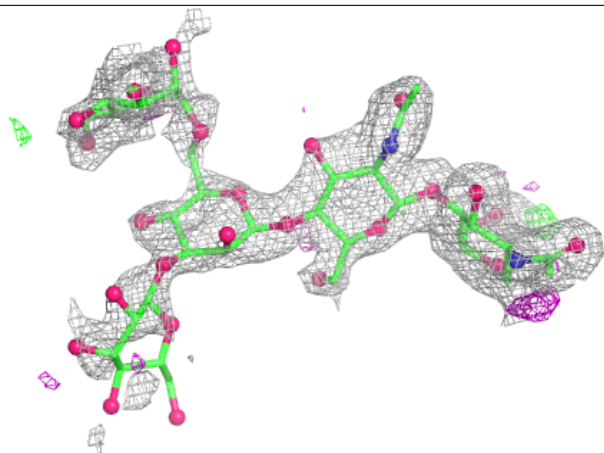
**Electron density around Chain E:**

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



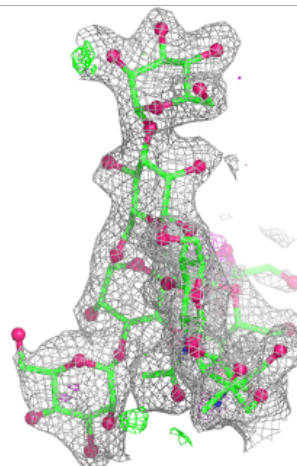
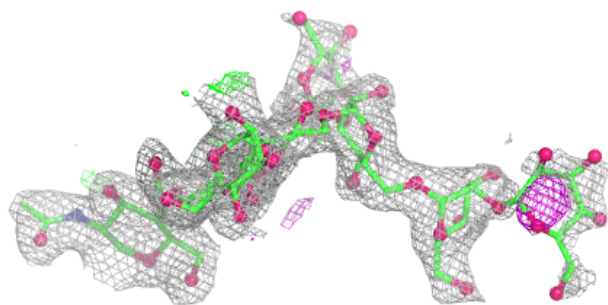
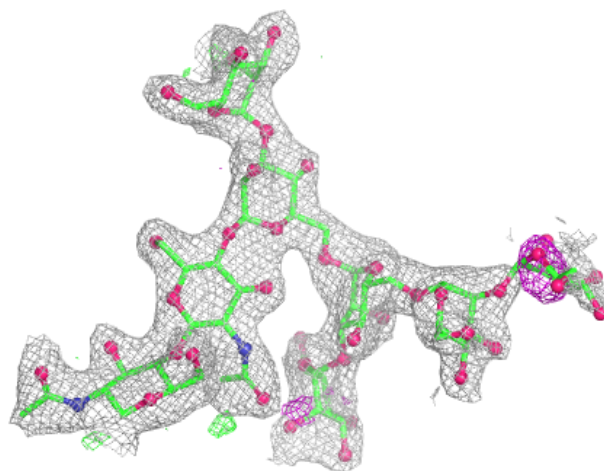
Electron density around Chain D:

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



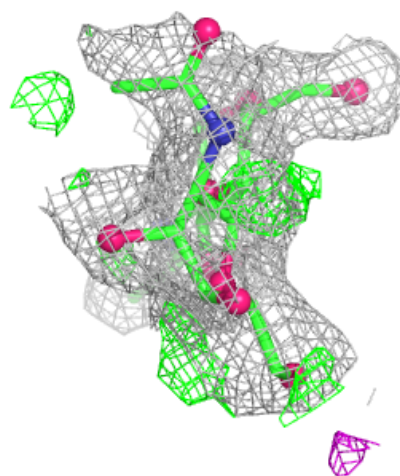
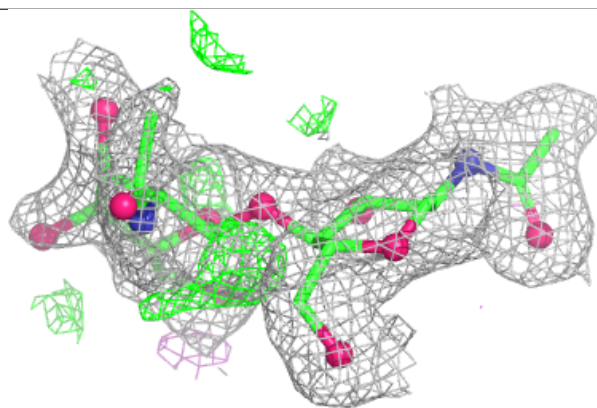
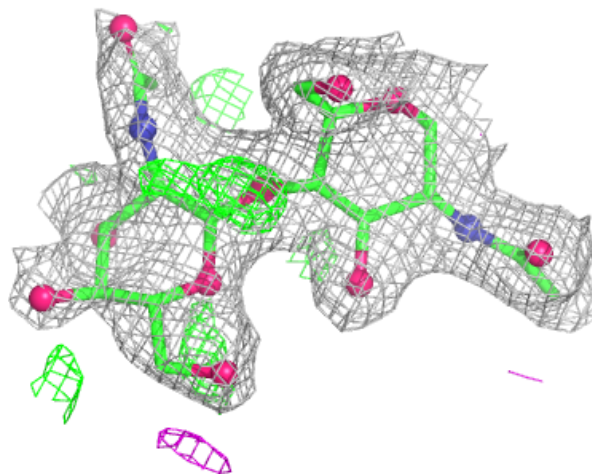
Electron density around Chain F:

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



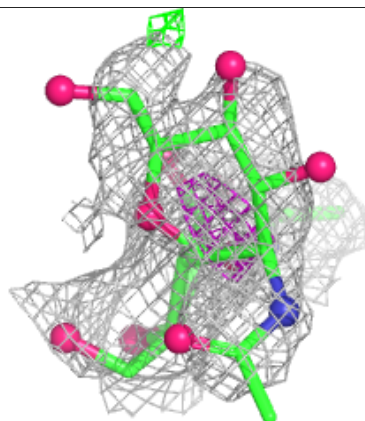
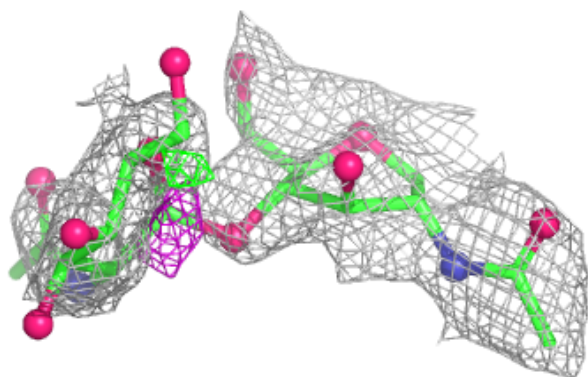
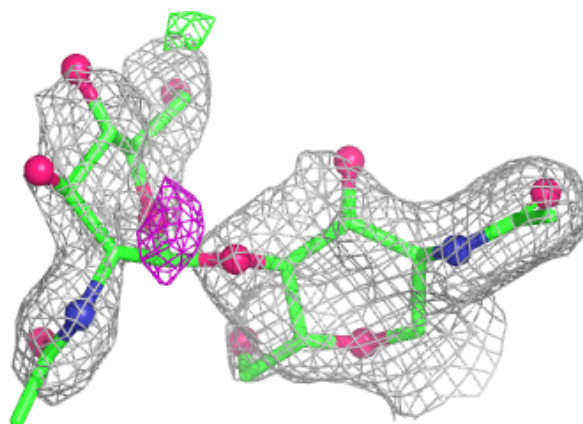
Electron density around Chain G:

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



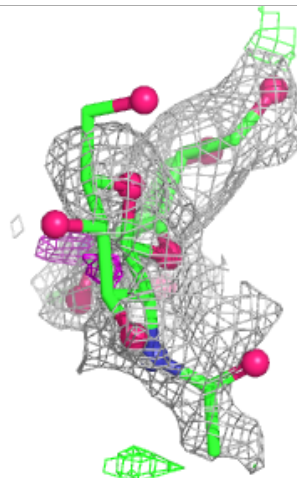
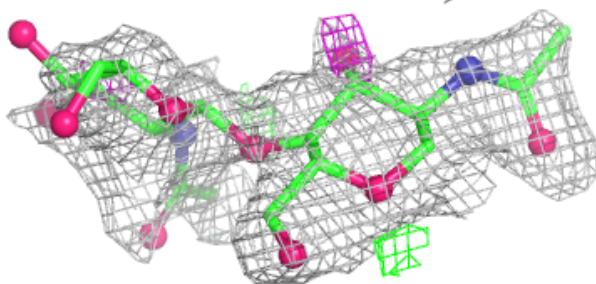
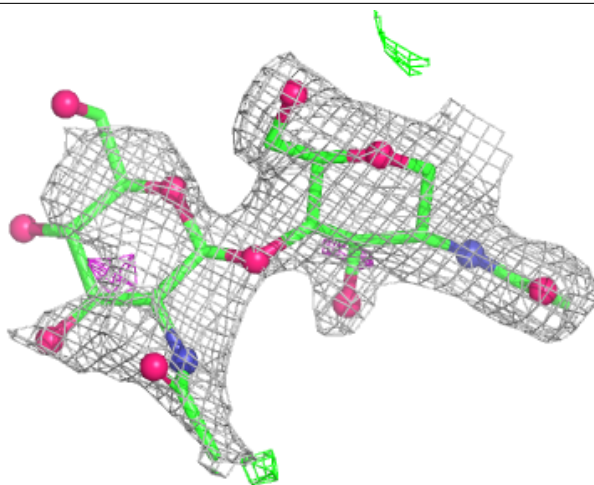
Electron density around Chain H:

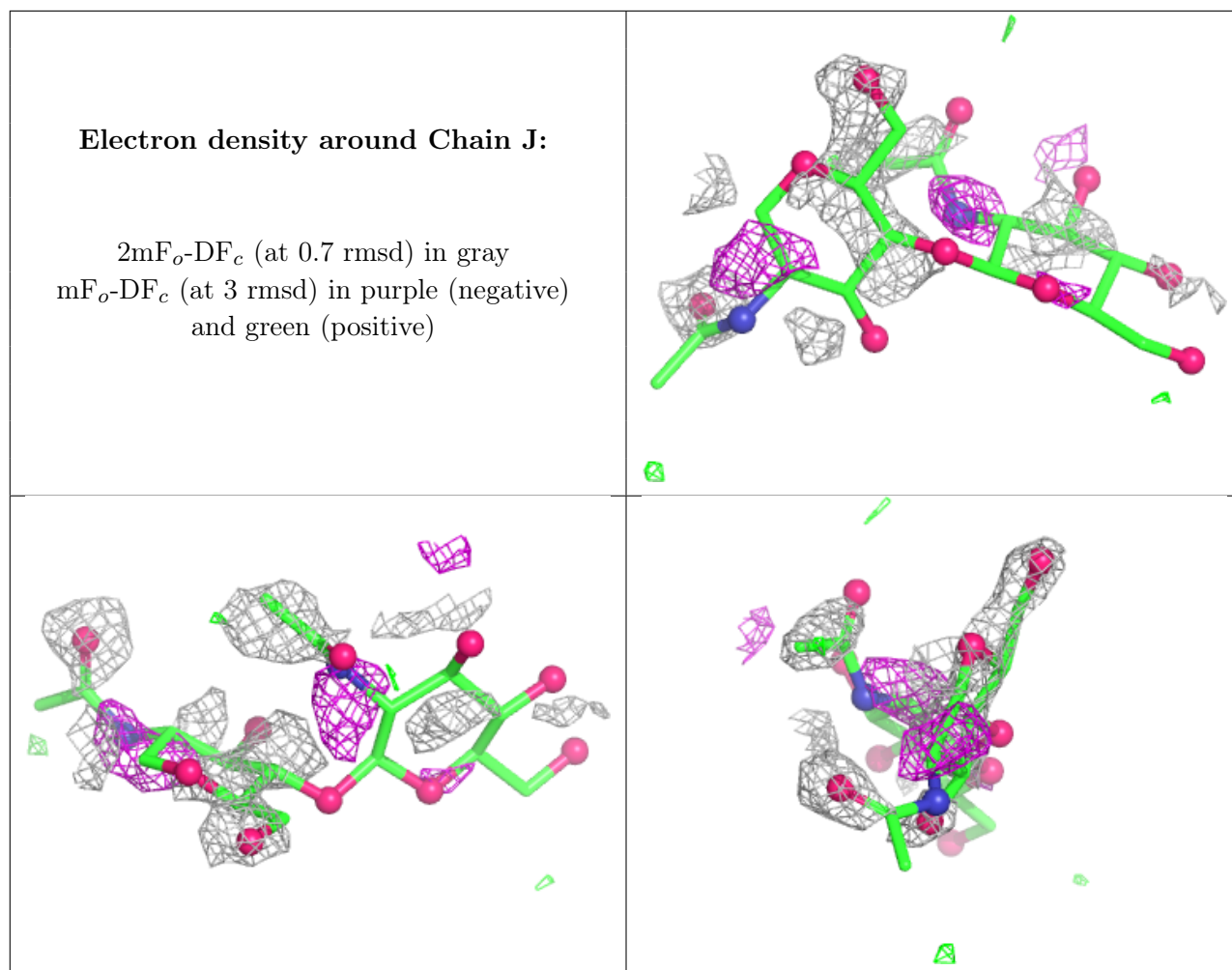
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

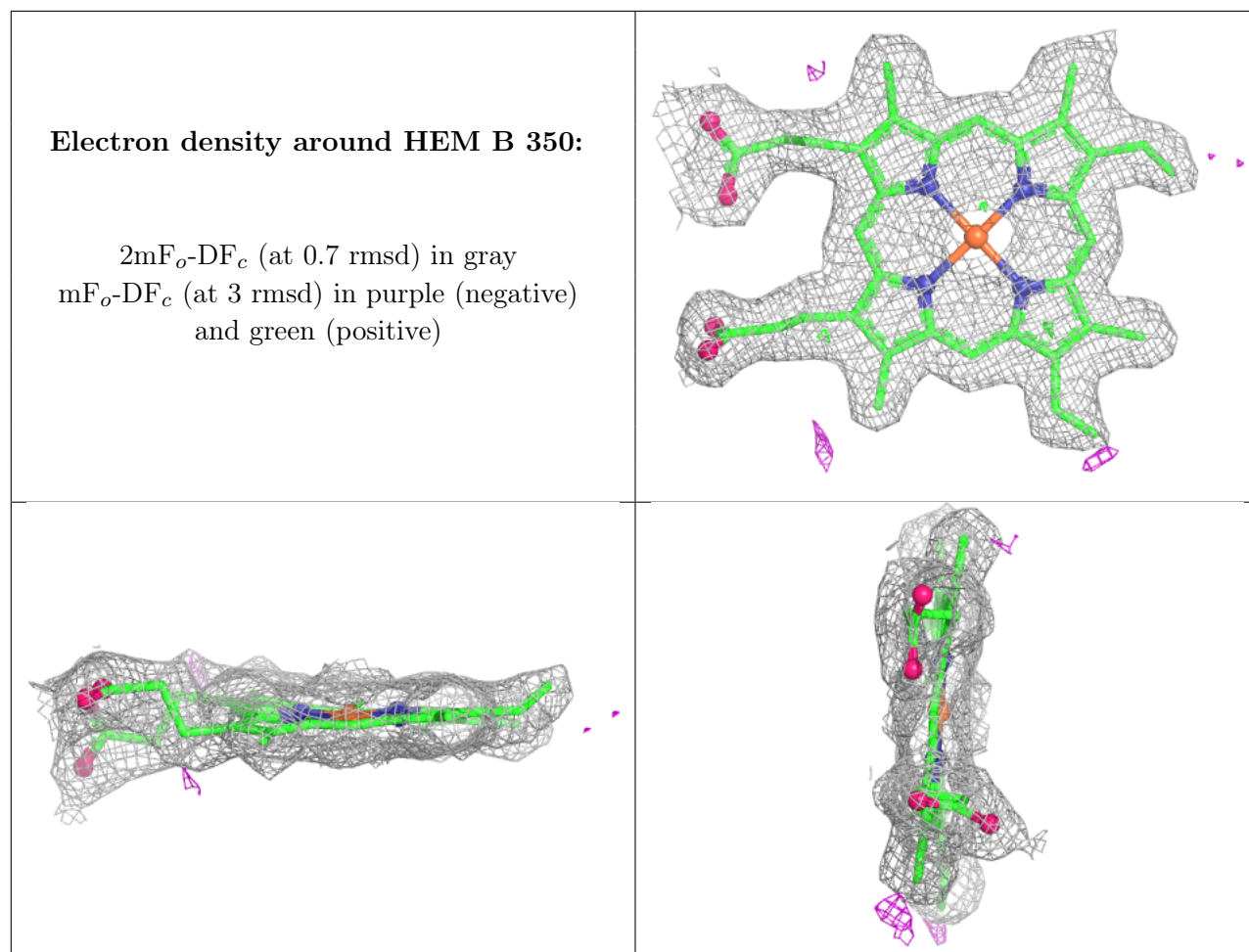
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	TRS	B	1355	8/8	0.58	0.47	88,89,90,90	0
9	NAG	B	411	14/15	0.62	0.66	71,77,81,81	0
10	BMA	B	501	12/12	0.66	0.36	48,55,57,57	0
9	NAG	A	401	14/15	0.68	0.47	66,70,72,73	0
9	NAG	A	391	14/15	0.70	0.28	39,54,65,66	0
9	NAG	B	511	15/15	0.71	0.40	48,54,60,61	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

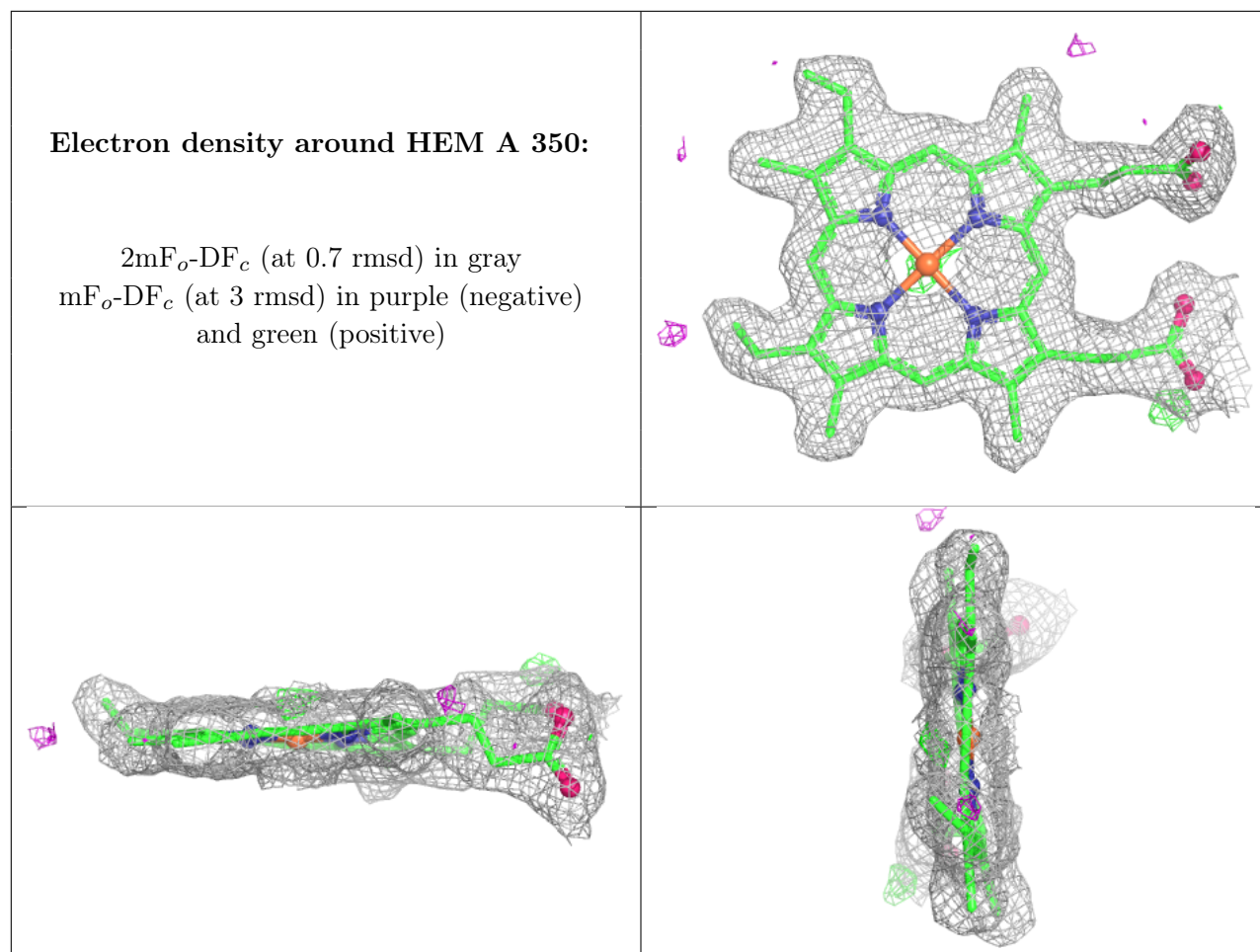
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	SO4	B	1359	5/5	0.94	0.27	68,68,70,72	0
11	SO4	A	1355	5/5	0.94	0.24	81,81,82,82	0
12	CL	B	1361	1/1	0.95	0.06	51,51,51,51	0
11	SO4	A	1358	5/5	0.96	0.14	75,76,77,77	0
8	MZ0	A	354	7/7	0.96	0.12	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.