



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:44 PM UTC

PDB ID : 4CUO / pdb\_00004cuo  
Title : Banyan peroxidase with glycosylation  
Authors : Palm, G.J.; Sharma, A.; Hinrichs, W.  
Deposited on : 2014-03-20  
Resolution : 1.67 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

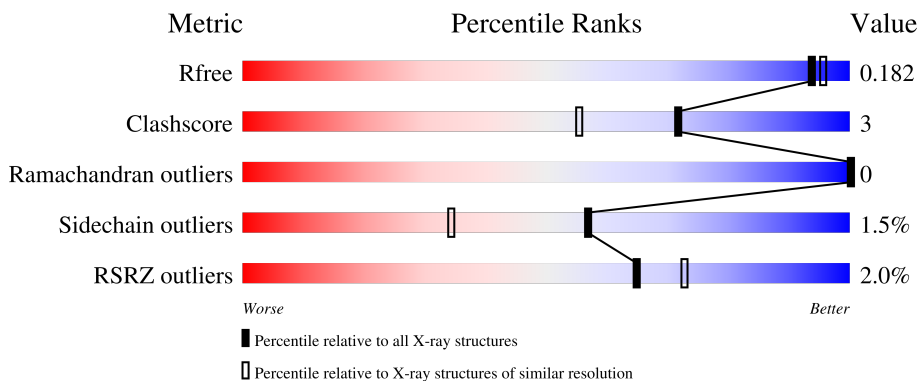
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.67 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	306	 2% 90% 9%
2	B	2	 50% 50%
3	C	7	 86% 14%
4	D	3	 100%
4	E	3	 100%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
11	CO3	A	1338	-	X	-	-
6	NAG	A	1320	X	-	-	-
6	NAG	A	1324	X	-	-	-

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 2989 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 BANYAN PEROXIDASE.

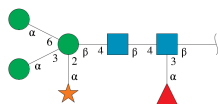
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	306	2360	1466	405	478	11	0	11	0

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



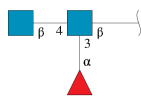
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	24	14	1	9	0	0	0

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



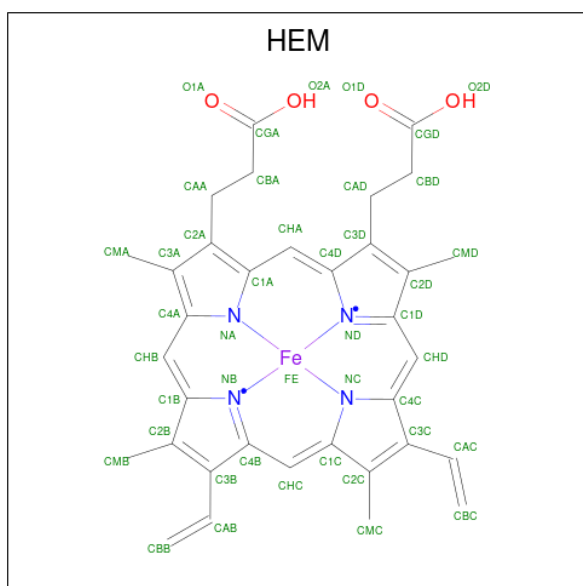
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	7	80	45	2	33	0	0	0

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



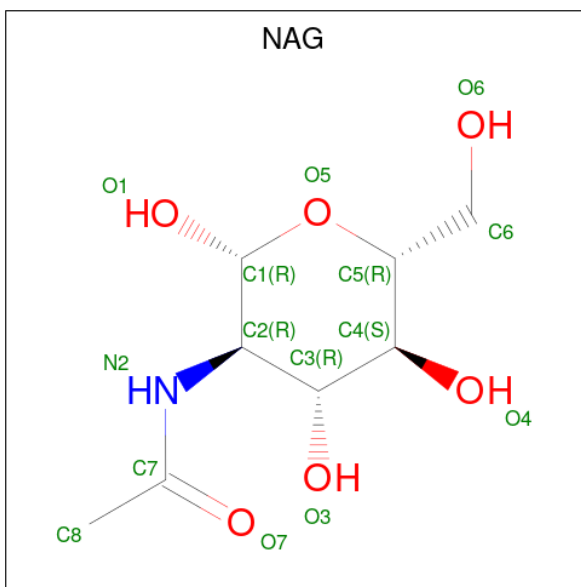
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	3	38	22	2	14	0	0	0
4	E	3	39	22	2	15	0	1	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	2	2	2	0	0

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
8	A	1	1	1	0	0

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

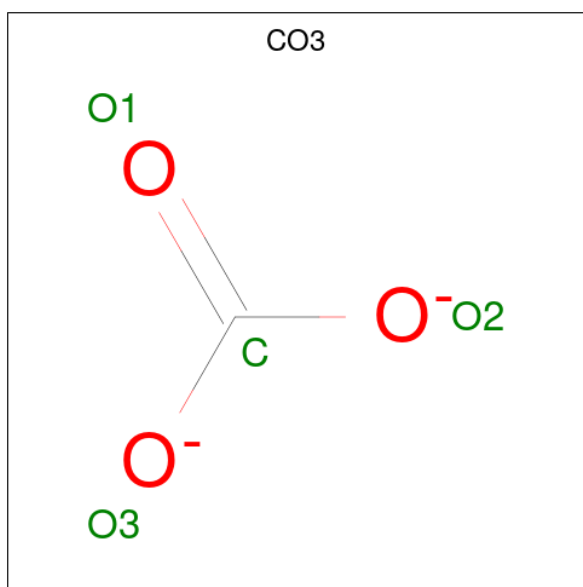
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
9	A	3	3	3	0	0

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 11 is CARBONATE ION (CCD ID: CO3) (formula: CO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 4 1 3	0	0
11	A	1	Total C O 4 1 3	0	0
11	A	1	Total C O 4 1 3	0	0

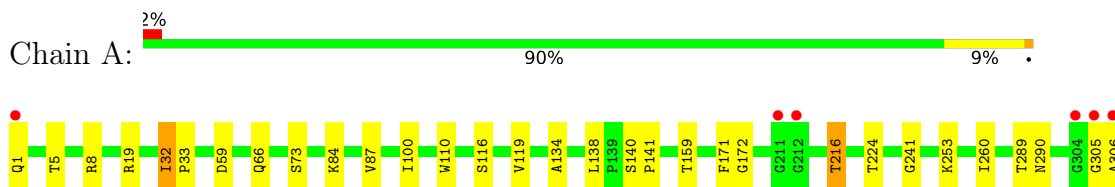
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	321	Total O 326 326	0	5

### 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.

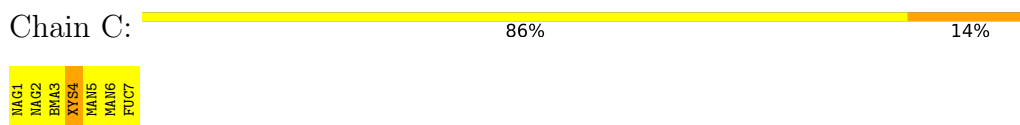
- Molecule 1: BANYAN PEROXIDASE



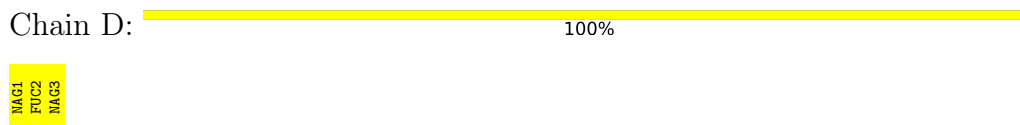
- Molecule 2: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



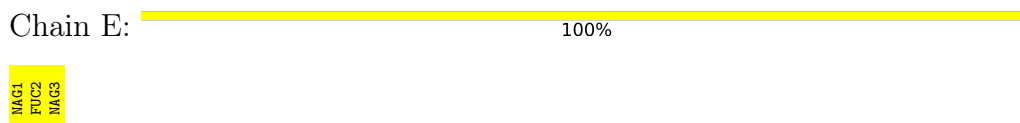
- Molecule 3: alpha-D-xylopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)][alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.11Å 73.11Å 164.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	63.32 – 1.67 63.32 – 1.67	Depositor EDS
% Data completeness (in resolution range)	99.6 (63.32-1.67) 99.7 (63.32-1.67)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 1.67Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.157 , 0.180 0.159 , 0.182	Depositor DCC
$R_{free}$ test set	3050 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtrriage
Anisotropy	0.508	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2989	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, CA, MAN, HEM, XY5, SNN, SO4, NA, FUC, CL, CO3

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	1.33	5/2418 (0.2%)	1.18	4/3290 (0.1%)

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	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	241	GLY	N-CA	6.25	1.52	1.45
1	A	119	VAL	N-CA	6.23	1.51	1.46
1	A	32	ILE	CA-CB	5.50	1.57	1.53
1	A	134	ALA	N-CA	5.27	1.52	1.46
1	A	224	THR	CA-C	5.08	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	PRO	N-CA-C	-5.97	108.47	114.68
1	A	216	THR	N-CA-C	-5.09	103.43	110.35
1	A	138	LEU	CA-C-N	-5.00	114.76	119.76
1	A	138	LEU	C-N-CA	-5.00	114.76	119.76

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289	THR	Mainchain

## 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	2360	0	2287	16	0
2	B	24	0	22	1	0
3	C	80	0	68	1	0
4	D	38	0	34	0	0
4	E	39	0	29	0	0
5	A	43	0	30	1	0
6	A	42	0	39	2	0
7	A	2	0	0	0	0
8	A	1	0	0	0	0
9	A	3	0	0	0	0
10	A	15	0	0	0	0
11	A	16	0	0	1	0
12	A	326	0	0	3	0
All	All	2989	0	2509	17	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 3.

All (17) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87[B]:VAL:HG21	1:A:100:ILE:HD11	1.69	0.74
1:A:253:LYS:HG2	12:A:2254:HOH:O	1.90	0.71
1:A:260:ILE:HD11	6:A:1325:NAG:H82	1.72	0.71
1:A:305[B]:GLY:O	1:A:306[B]:ALA:HB2	1.93	0.68
12:A:2312:HOH:O	3:C:4:XY5:H51	1.96	0.65
1:A:5:THR:HB	1:A:8:ARG:HD3	1.91	0.52
1:A:305[B]:GLY:O	1:A:306[B]:ALA:CB	2.58	0.52
1:A:59[A]:ASP:HB2	1:A:306[A]:ALA:CB	2.41	0.51
1:A:159:THR:HG21	6:A:1325:NAG:C1	2.46	0.46
1:A:19:ARG:NH1	11:A:1335:CO3:O2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ILE:CG2	1:A:33:PRO:HD3	2.47	0.44
1:A:73:SER:HB2	12:A:2100:HOH:O	2.18	0.43
1:A:110:TRP:CD1	1:A:116:SER:HB3	2.53	0.42
1:A:172:GLY:HA3	5:A:1307:HEM:HAD1	2.00	0.42
1:A:84:LYS:HA	1:A:87[B]:VAL:HG22	2.03	0.41
1:A:253:LYS:HA	1:A:253:LYS:HD3	1.97	0.41
1:A:66:GLN:HB3	2:B:1:NAG:H82	2.03	0.41

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	312/306 (102%)	306 (98%)	6 (2%)	0	100 100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	268/260 (103%)	264 (98%)	4 (2%)	57 34

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	140	SER
1	A	171	PHE
1	A	216	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	23	GLN
1	A	47	ASN
1	A	72	ASN
1	A	136	GLN
1	A	210	GLN
1	A	239	GLN
1	A	273	ASN
1	A	284	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](#)

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
1	SNN	A	290	1	7,8,8	6.95	2 (28%)	10,11,11	7.43	7 (70%)

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
1	SNN	A	290	1	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	290	SNN	C5-N1	14.32	1.60	1.37
1	A	290	SNN	C-N1	11.32	1.52	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	SNN	C5-N1-C	-16.79	97.08	113.96
1	A	290	SNN	CA-C-N1	13.79	118.12	107.30
1	A	290	SNN	O-C-N1	-6.20	117.62	124.93
1	A	290	SNN	C4-C5-N1	4.58	113.46	108.02
1	A	290	SNN	O-C-CA	-2.70	124.24	126.19
1	A	290	SNN	CA-C4-C5	2.23	106.16	103.55
1	A	290	SNN	O5-C5-N1	-2.20	122.13	125.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates i

16 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	B	1	1,2	14,14,15	0.73	0	17,19,21	2.16	3 (17%)
2	FUC	B	2	2	10,10,11	0.62	0	14,14,16	0.59	0
3	NAG	C	1	1,3	14,14,15	0.83	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
3	NAG	C	2	3	14,14,15	0.90	1 (7%)	17,19,21	1.46	2 (11%)
3	BMA	C	3	3	11,11,12	1.11	1 (9%)	15,15,17	1.10	2 (13%)
3	XYS	C	4	3	9,9,10	1.62	2 (22%)	10,12,14	2.09	4 (40%)
3	MAN	C	5	3	11,11,12	0.78	1 (9%)	15,15,17	1.71	4 (26%)
3	MAN	C	6	3	11,11,12	0.62	0	15,15,17	1.65	2 (13%)
3	FUC	C	7	3	10,10,11	1.20	1 (10%)	14,14,16	1.05	1 (7%)
4	NAG	D	1	1,4	14,14,15	0.80	0	17,19,21	1.28	3 (17%)
4	FUC	D	2	4	10,10,11	0.74	0	14,14,16	1.05	1 (7%)
4	NAG	D	3	4	14,14,15	0.56	0	17,19,21	1.14	1 (5%)
4	NAG	E	1[A]	-	14,14,15	0.79	1 (7%)	17,19,21	1.79	4 (23%)
4	NAG	E	1[B]	-	14,14,15	0.80	1 (7%)	17,19,21	1.81	4 (23%)
4	FUC	E	2	4	10,10,11	0.59	0	14,14,16	0.92	1 (7%)
4	NAG	E	3	4	14,14,15	0.52	0	17,19,21	1.87	4 (23%)

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	B	1	1,2	-	2/6/23/26	0/1/1/1
2	FUC	B	2	2	-	-	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	XYS	C	4	3	-	-	0/1/1/1
3	MAN	C	5	3	-	2/2/19/22	0/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
3	FUC	C	7	3	-	-	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	FUC	D	2	4	-	-	0/1/1/1
4	NAG	D	3	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1[A]	-	-	0/6/23/26	0/1/1/1
4	NAG	E	1[B]	-	-	0/6/23/26	0/1/1/1
4	FUC	E	2	4	-	-	0/1/1/1
4	NAG	E	3	4	-	2/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	XYS	O5-C1	3.22	1.49	1.43
3	C	3	BMA	O2-C2	3.09	1.49	1.43
3	C	4	XYS	C2-C3	2.91	1.56	1.52
3	C	7	FUC	C2-C3	2.63	1.56	1.52
3	C	2	NAG	O5-C5	-2.19	1.39	1.43
3	C	5	MAN	C2-C3	2.05	1.55	1.52
4	E	1[A]	NAG	O7-C7	2.01	1.27	1.23
4	E	1[B]	NAG	O7-C7	2.01	1.27	1.23

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C2-N2-C7	-6.05	114.79	122.90
4	E	1[A]	NAG	O5-C1-C2	-4.85	103.79	111.29
4	E	1[B]	NAG	O5-C1-C2	-4.85	103.79	111.29
2	B	1	NAG	C1-O5-C5	4.74	118.54	112.19
3	C	6	MAN	C1-O5-C5	4.56	118.30	112.19
4	E	3	NAG	C1-O5-C5	4.56	118.30	112.19
3	C	4	XYS	C1-C2-C3	4.45	116.12	109.64
4	E	3	NAG	C2-N2-C7	3.79	127.98	122.90
3	C	1	NAG	C2-N2-C7	-3.39	118.36	122.90
3	C	5	MAN	O2-C2-C3	3.36	117.11	110.15
3	C	2	NAG	C1-O5-C5	3.19	116.46	112.19
3	C	5	MAN	C1-O5-C5	3.07	116.30	112.19
3	C	1	NAG	O3-C3-C4	-2.87	103.61	110.38
3	C	4	XYS	C4-C3-C2	2.76	114.20	110.92
4	E	1[A]	NAG	C4-C3-C2	-2.69	107.07	111.02
4	E	1[B]	NAG	C4-C3-C2	-2.69	107.07	111.02
4	E	1[A]	NAG	O5-C5-C4	-2.68	104.30	110.83
4	E	1[B]	NAG	O5-C5-C4	-2.68	104.30	110.83
3	C	2	NAG	O5-C1-C2	-2.64	107.21	111.29
4	E	1[A]	NAG	C3-C4-C5	-2.56	105.60	110.23
4	E	1[B]	NAG	C3-C4-C5	-2.56	105.60	110.23
3	C	6	MAN	O2-C2-C1	2.40	114.71	109.22
3	C	1	NAG	C1-C2-N2	-2.29	106.83	110.43
3	C	5	MAN	O5-C5-C6	2.28	112.11	107.66
3	C	4	XYS	C5-O5-C1	-2.23	107.81	111.42
4	E	3	NAG	O7-C7-N2	2.23	125.92	121.98
3	C	5	MAN	C1-C2-C3	-2.21	106.43	109.64
4	D	1	NAG	O6-C6-C5	-2.13	104.10	111.33
4	D	2	FUC	O5-C5-C4	2.11	113.35	109.55
3	C	7	FUC	C1-C2-C3	-2.11	106.58	109.64
3	C	3	BMA	C1-C2-C3	-2.10	106.59	109.64

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3	NAG	O7-C7-N2	2.10	125.69	121.98
3	C	1	NAG	C4-C3-C2	2.09	114.08	111.02
4	D	1	NAG	C8-C7-N2	-2.08	112.66	116.12
3	C	4	XYS	O3-C3-C2	2.05	114.25	110.05
4	D	1	NAG	C1-O5-C5	2.05	114.94	112.19
4	E	2	FUC	C3-C4-C5	2.04	112.92	109.81
3	C	3	BMA	O5-C5-C6	-2.03	103.71	107.66
4	E	3	NAG	O5-C1-C2	2.02	114.42	111.29
2	B	1	NAG	O3-C3-C4	-2.01	105.64	110.38

There are no chirality outliers.

All (8) torsion outliers are listed below:

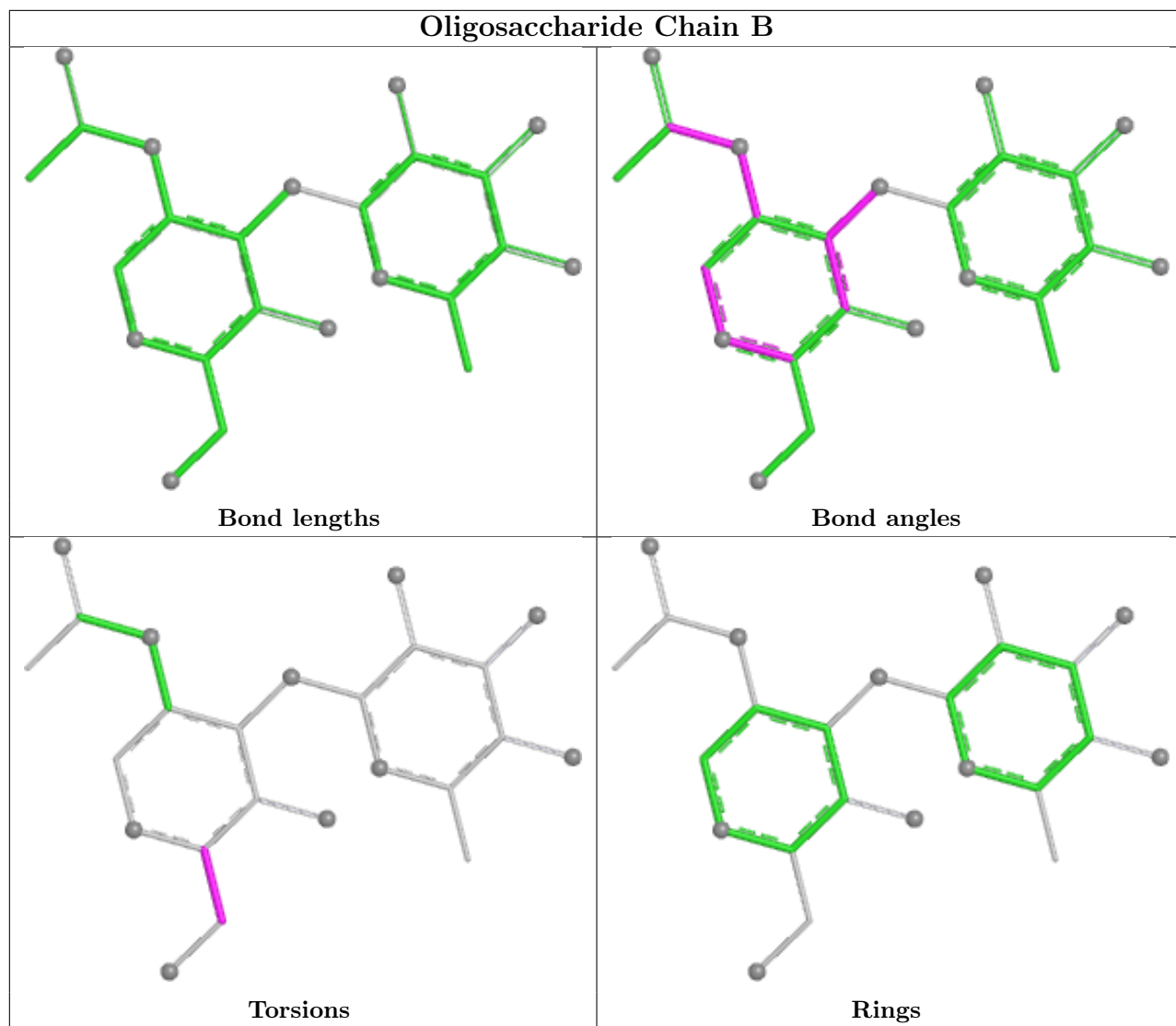
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
4	E	3	NAG	C4-C5-C6-O6
3	C	5	MAN	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
3	C	5	MAN	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	E	3	NAG	O5-C5-C6-O6

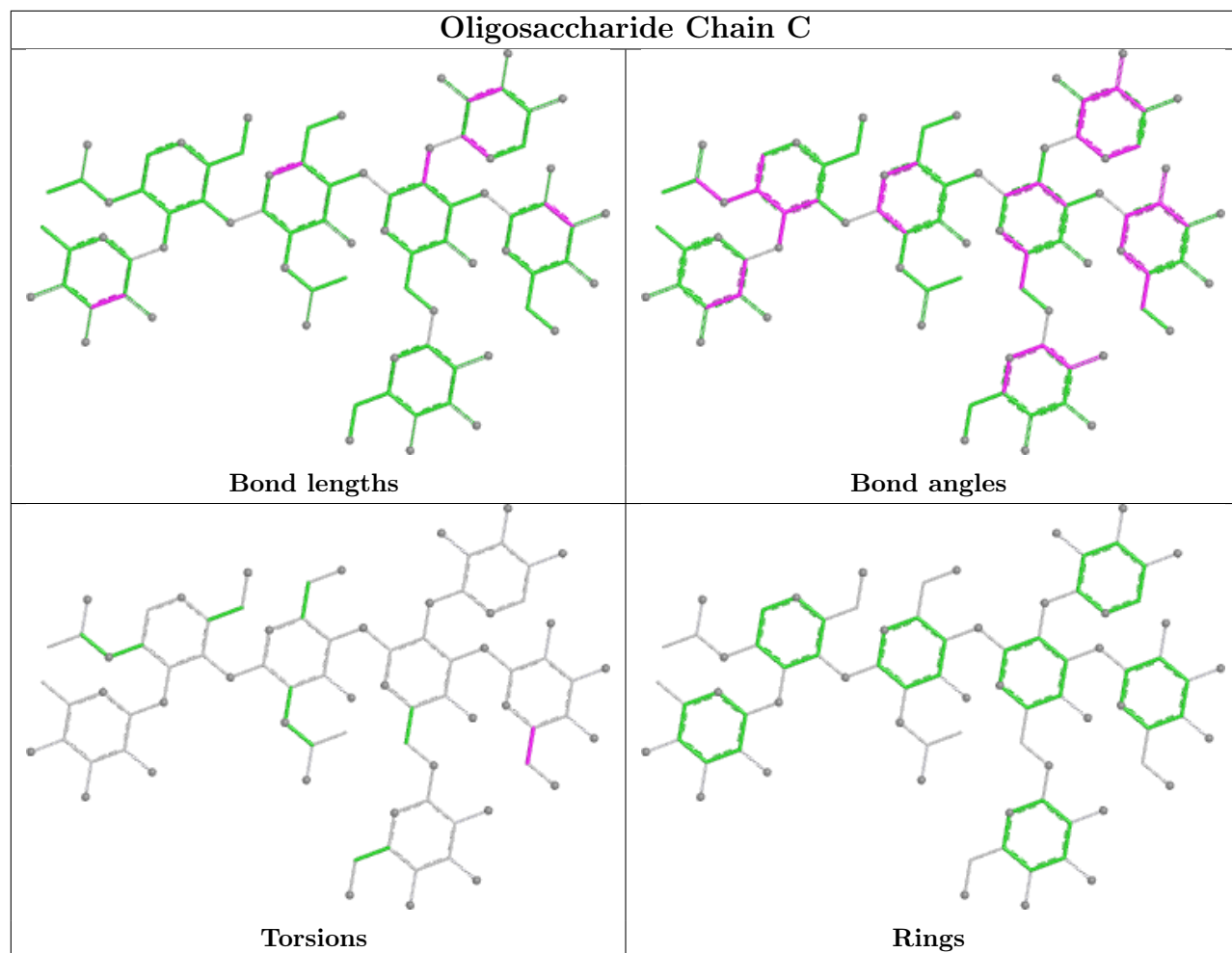
There are no ring outliers.

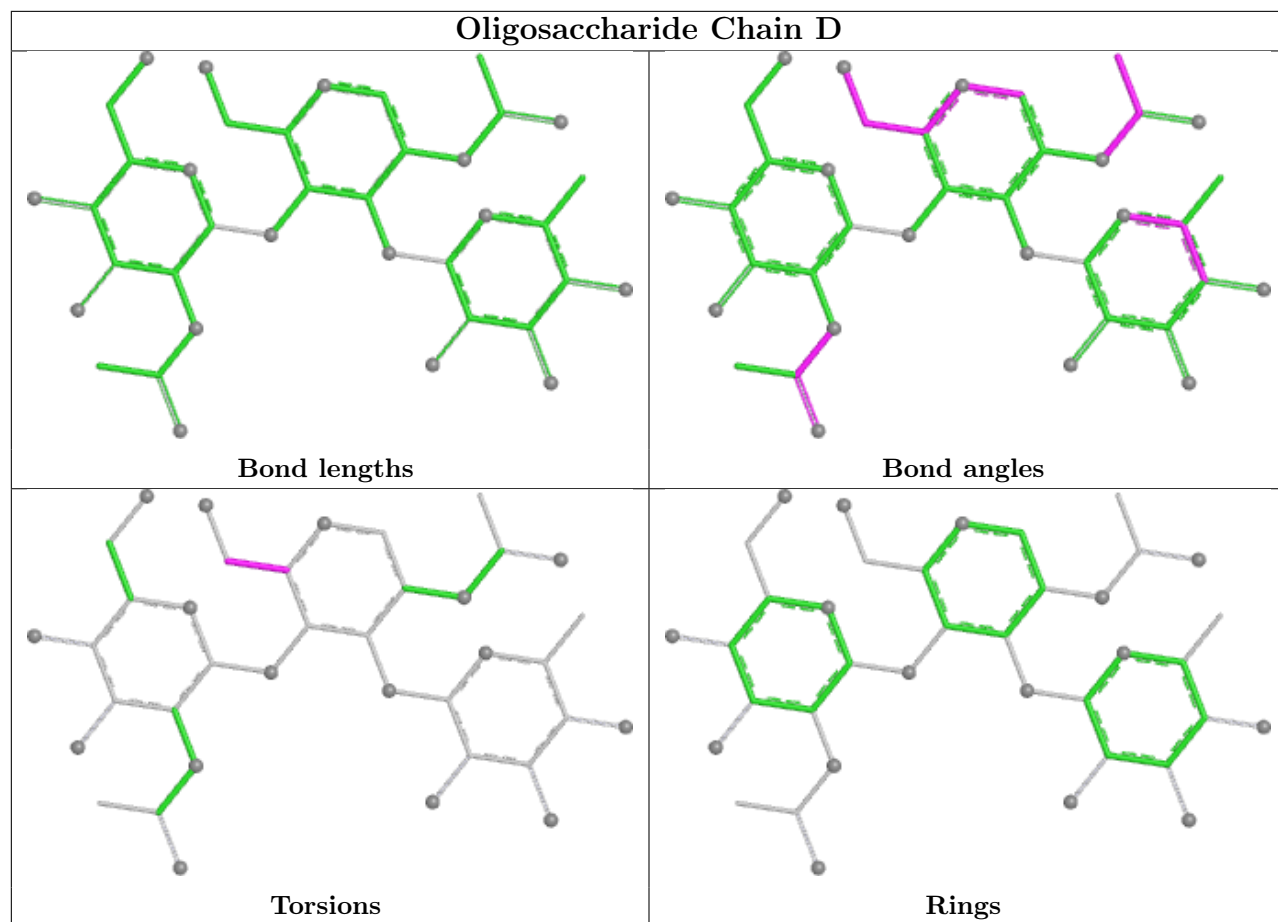
2 monomers are involved in 2 short contacts:

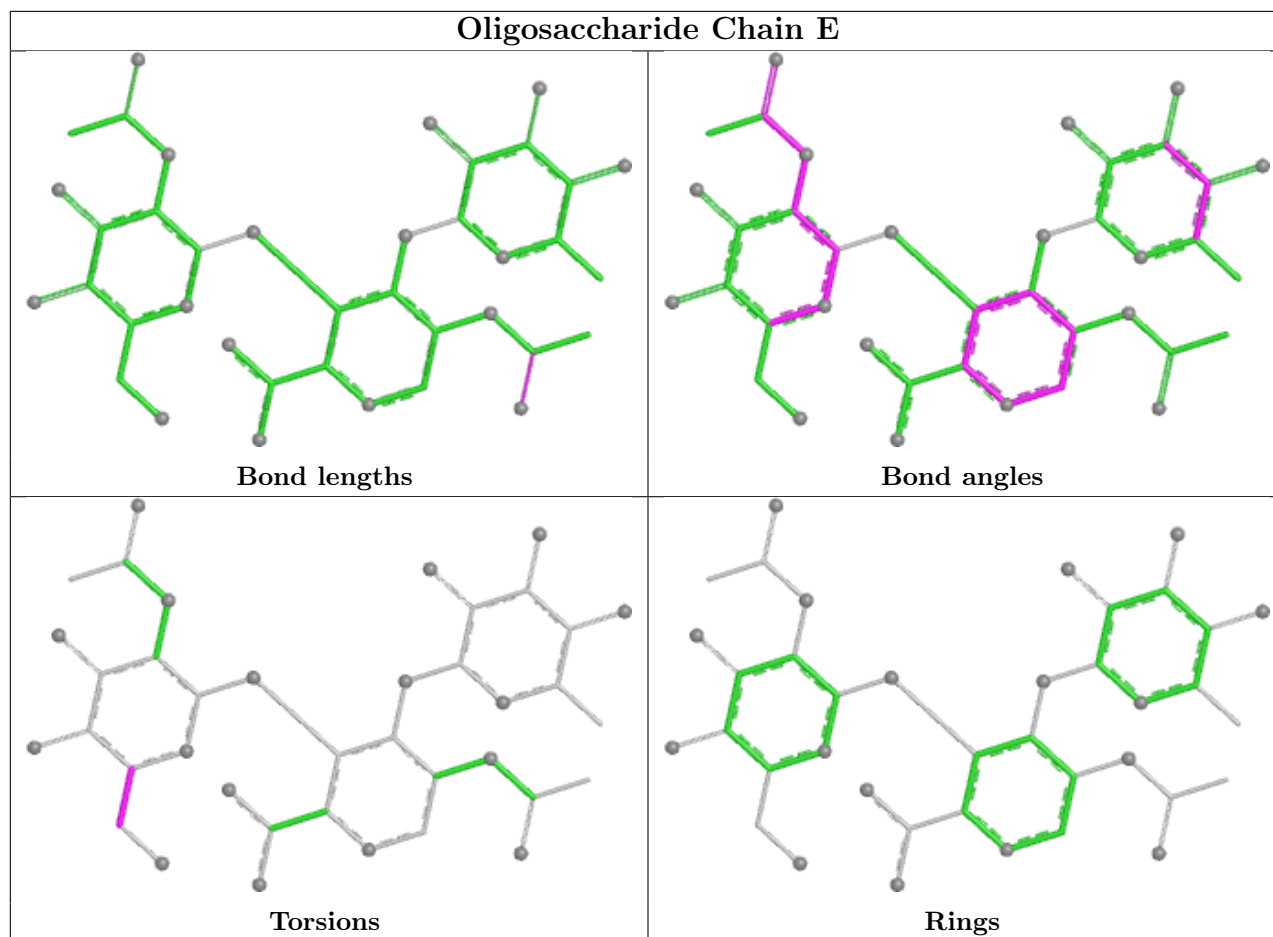
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	4	XYS	1	0
2	B	1	NAG	1	0

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









## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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$
6	NAG	A	1324	1	14,14,15	0.78	1 (7%)	17,19,21	1.27	2 (11%)
6	NAG	A	1320	1	14,14,15	0.65	0	17,19,21	1.30	3 (17%)
10	SO4	A	1333	-	4,4,4	0.41	0	6,6,6	0.96	1 (16%)
10	SO4	A	1332	-	4,4,4	0.54	0	6,6,6	0.55	0
11	CO3	A	1335	-	3,3,3	1.18	0	2,3,3	0.58	0
11	CO3	A	1338	-	3,3,3	2.27	2 (66%)	2,3,3	4.83	2 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	CO3	A	1336	-	3,3,3	1.16	0	2,3,3	1.08	0
6	NAG	A	1325	1	14,14,15	0.95	2 (14%)	17,19,21	2.90	5 (29%)
5	HEM	A	1307	1	50,50,50	1.71	12 (24%)	67,82,82	1.59	11 (16%)
11	CO3	A	1337	-	3,3,3	1.28	0	2,3,3	0.44	0
10	SO4	A	1334	-	4,4,4	0.51	0	6,6,6	0.29	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
6	NAG	A	1324	1	1/1/5/7	3/6/23/26	0/1/1/1
6	NAG	A	1320	1	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	A	1325	1	-	0/6/23/26	0/1/1/1
5	HEM	A	1307	1	-	2/14/54/54	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1307	HEM	FE-NB	4.19	2.07	1.94
5	A	1307	HEM	FE-NC	3.90	2.08	1.95
5	A	1307	HEM	O1A-CGA	3.26	1.32	1.22
11	A	1338	CO3	O1-C	-3.10	1.15	1.25
5	A	1307	HEM	O1D-CGD	2.99	1.31	1.22
5	A	1307	HEM	CMB-C2B	2.90	1.56	1.50
5	A	1307	HEM	FE-NA	2.82	2.04	1.95
5	A	1307	HEM	FE-ND	2.70	2.03	1.94
5	A	1307	HEM	CMC-C2C	2.44	1.55	1.50
11	A	1338	CO3	O3-C	-2.37	1.13	1.33
5	A	1307	HEM	C1B-NB	-2.35	1.36	1.40
5	A	1307	HEM	C4D-ND	-2.34	1.36	1.40
6	A	1324	NAG	C1-C2	2.29	1.55	1.52
6	A	1325	NAG	C1-C2	2.17	1.55	1.52
5	A	1307	HEM	CHA-C4D	2.06	1.42	1.38
6	A	1325	NAG	C2-N2	2.02	1.49	1.46
5	A	1307	HEM	CHC-C4B	2.02	1.43	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1325	NAG	C1-O5-C5	7.69	122.50	112.19
6	A	1325	NAG	O5-C1-C2	6.76	121.75	111.29
11	A	1338	CO3	O3-C-O1	-6.14	103.98	119.68
5	A	1307	HEM	CHA-C4D-ND	4.77	130.26	124.37
6	A	1324	NAG	C2-N2-C7	3.97	128.22	122.90
5	A	1307	HEM	CHC-C4B-NB	3.96	128.69	124.42
5	A	1307	HEM	CHD-C4C-NC	3.90	128.70	124.45
5	A	1307	HEM	CHA-C4D-C3D	-3.39	118.98	125.23
6	A	1325	NAG	O7-C7-C8	-3.04	116.63	122.05
11	A	1338	CO3	O2-C-O1	2.99	127.33	119.68
5	A	1307	HEM	C3B-C2B-C1B	2.95	108.63	106.41
6	A	1325	NAG	C4-C3-C2	-2.82	106.88	111.02
5	A	1307	HEM	CHB-C4A-NA	2.78	128.90	123.86
5	A	1307	HEM	CBD-CAD-C3D	-2.76	104.89	112.53
6	A	1320	NAG	C1-O5-C5	2.62	115.70	112.19
6	A	1325	NAG	C2-N2-C7	2.62	126.41	122.90
5	A	1307	HEM	C4B-C3B-C2B	-2.58	104.91	107.28
6	A	1320	NAG	O5-C5-C6	2.47	112.46	107.66
6	A	1320	NAG	C1-C2-N2	-2.41	106.63	110.43
6	A	1324	NAG	C1-C2-N2	2.32	114.09	110.43
5	A	1307	HEM	O1A-CGA-CBA	-2.30	115.79	123.09
10	A	1333	SO4	O3-S-O2	2.13	120.68	109.56
5	A	1307	HEM	C4D-ND-C1D	2.06	107.65	105.21
5	A	1307	HEM	CBA-CAA-C2A	-2.05	106.86	112.53

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1320	NAG	C1
6	A	1324	NAG	C1

All (7) torsion outliers are listed below:

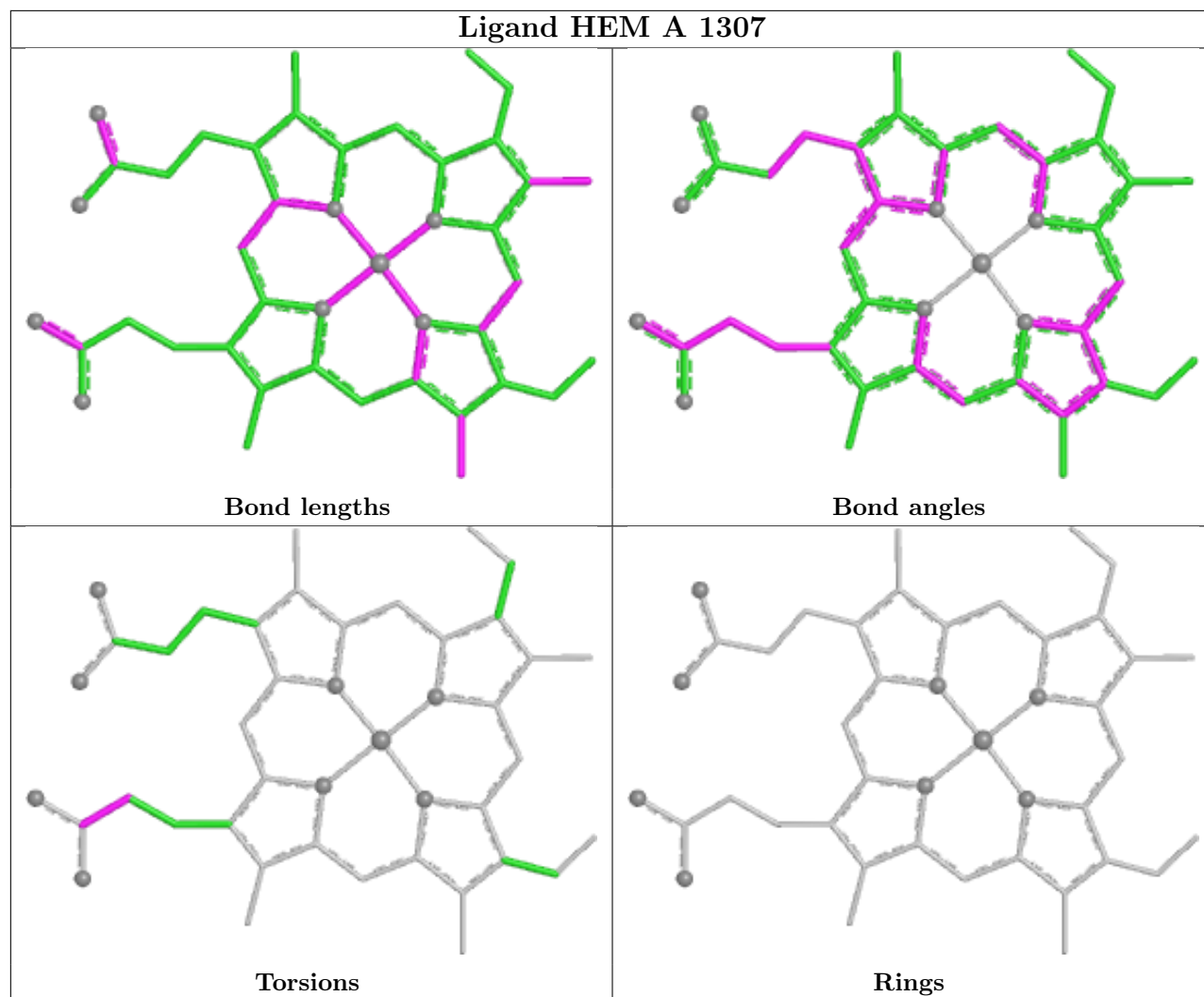
Mol	Chain	Res	Type	Atoms
6	A	1324	NAG	C4-C5-C6-O6
6	A	1324	NAG	O5-C5-C6-O6
6	A	1320	NAG	C4-C5-C6-O6
6	A	1320	NAG	O5-C5-C6-O6
6	A	1324	NAG	C1-C2-N2-C7
5	A	1307	HEM	CAA-CBA-CGA-O1A
5	A	1307	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1335	CO3	1	0
6	A	1325	NAG	2	0
5	A	1307	HEM	1	0

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



## 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	305/306 (99%)	-0.24	6 (1%) 65 73	21, 35, 51, 80	11 (3%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	306[A]	ALA	8.2
1	A	211	GLY	3.0
1	A	1	GLN	3.0
1	A	212	GLY	3.0
1	A	304	GLY	3.0
1	A	305[A]	GLY	2.9

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SNN	A	290	8/8	0.98	0.06	37,38,44,46	0

### 6.3 Carbohydrates [i](#)

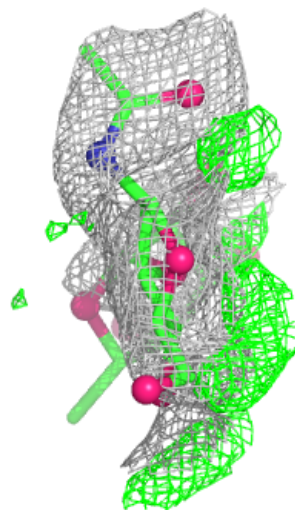
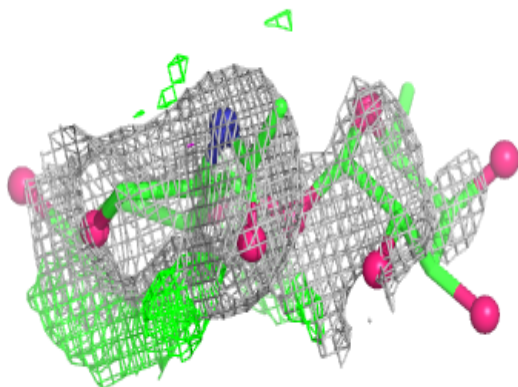
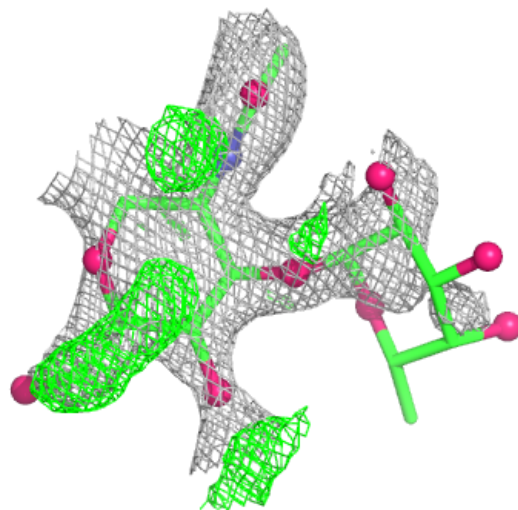
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FUC	B	2	10/11	0.72	0.21	92,97,100,101	10
2	NAG	B	1	14/15	0.76	0.18	55,74,83,84	14
4	NAG	E	3	14/15	0.77	0.14	80,94,110,112	0
3	MAN	C	5	11/12	0.78	0.12	60,70,80,82	0
4	NAG	D	3	14/15	0.80	0.12	90,100,107,110	0
4	FUC	D	2	10/11	0.83	0.13	90,99,104,104	0
4	NAG	D	1	14/15	0.84	0.10	60,67,79,83	0
4	FUC	E	2	10/11	0.85	0.13	61,73,79,80	0
3	MAN	C	6	11/12	0.88	0.10	52,57,61,62	0
3	XYS	C	4	9/10	0.88	0.10	55,66,73,76	0
4	NAG	E	1[A]	14/15	0.95	0.07	38,43,56,75	1
4	NAG	E	1[B]	14/15	0.95	0.07	38,43,56,75	1
3	NAG	C	2	14/15	0.96	0.07	40,42,45,46	0
3	BMA	C	3	11/12	0.96	0.06	42,45,50,52	0
3	NAG	C	1	14/15	0.96	0.07	35,38,45,48	0
3	FUC	C	7	10/11	0.97	0.06	38,39,40,41	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.

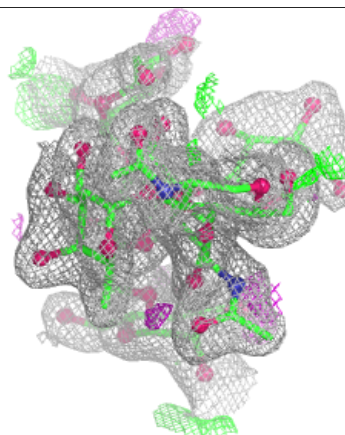
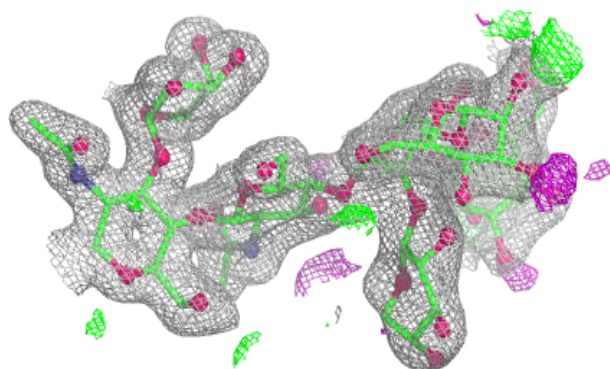
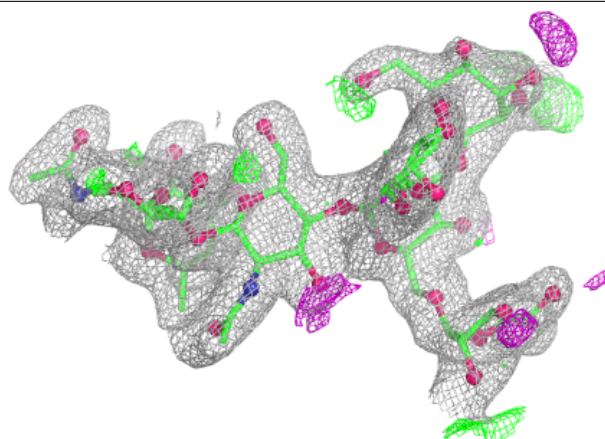
**Electron density around Chain B:**

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



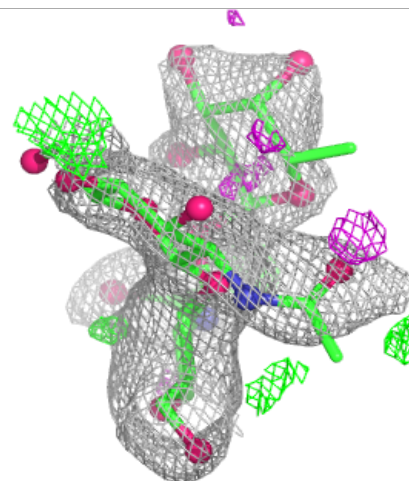
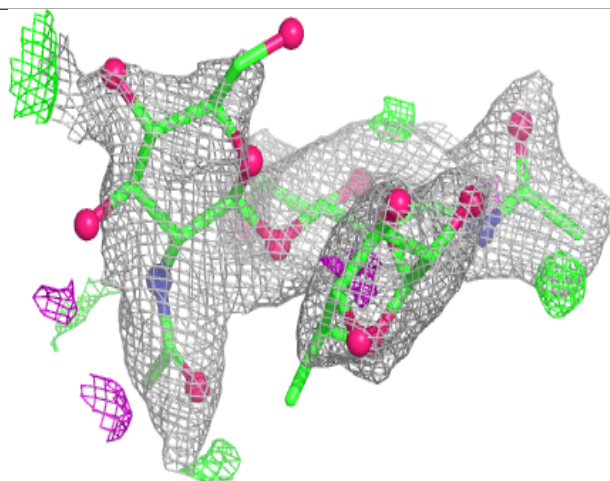
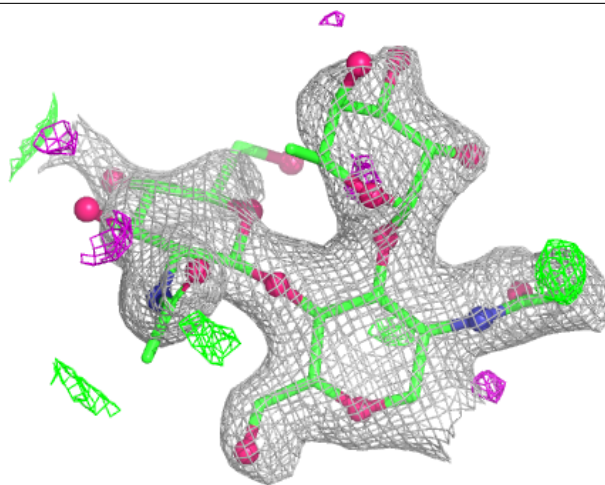
**Electron density around Chain C:**

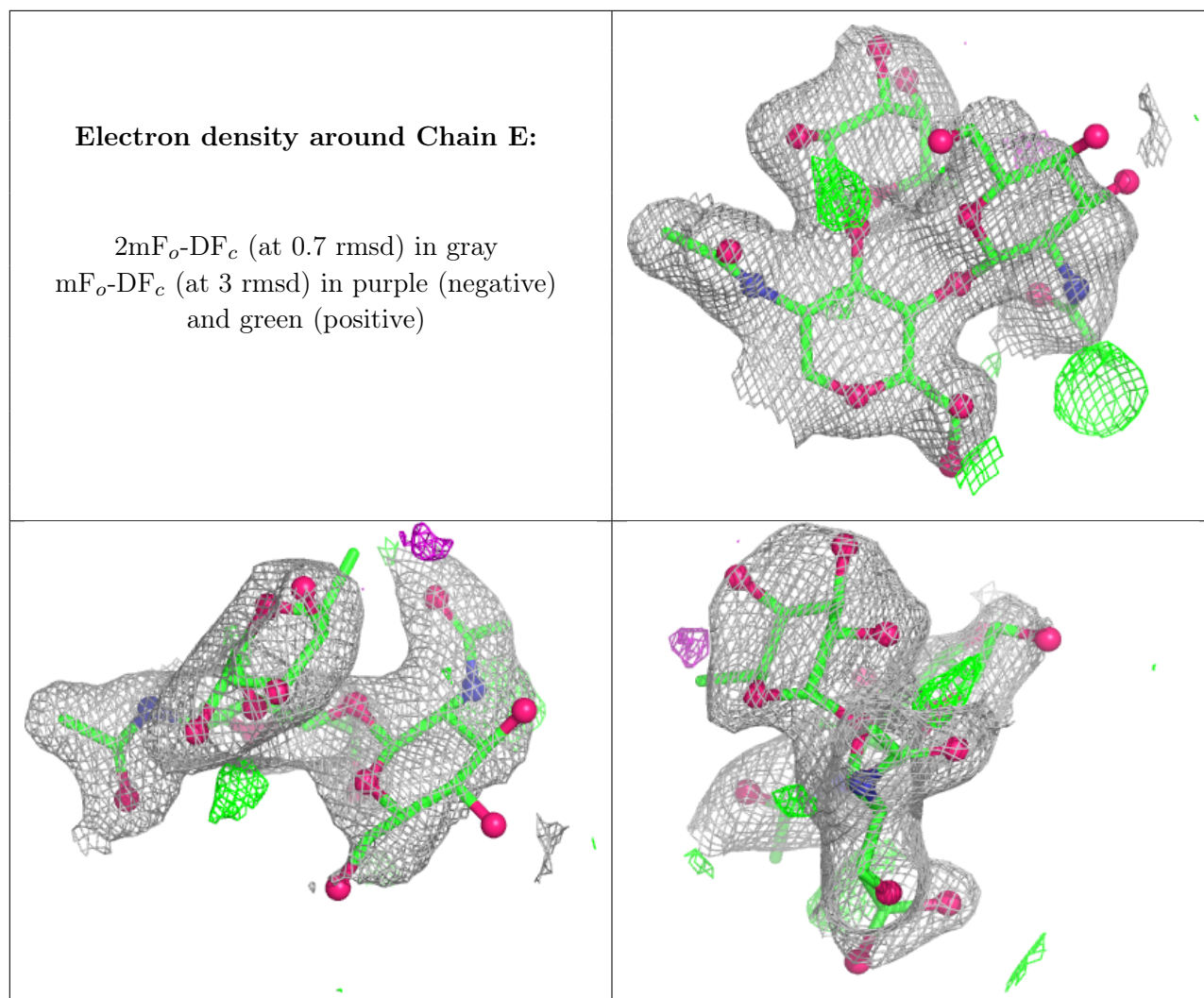
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain D:**

$2mF_o-DF_c$  (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.

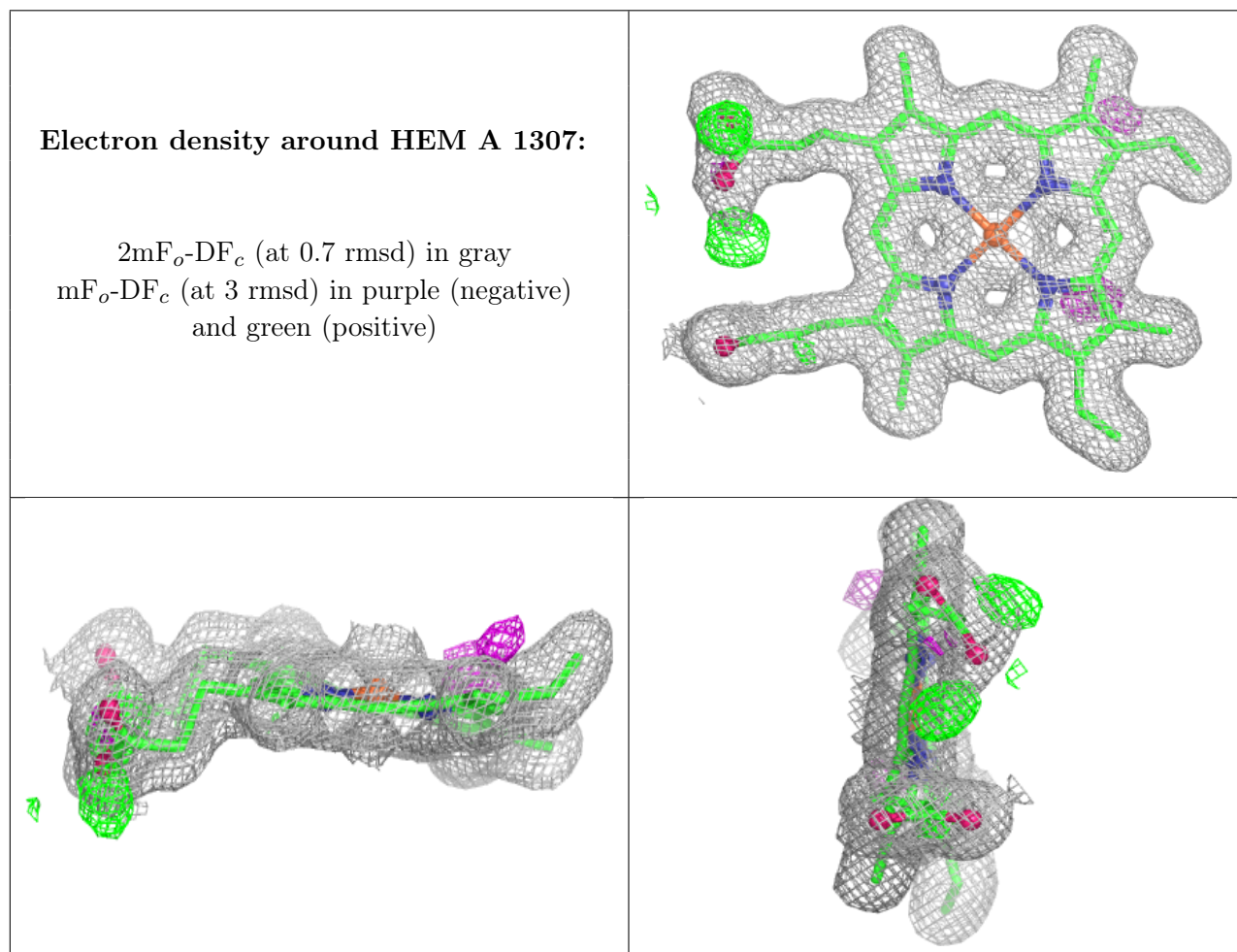
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	A	1320	14/15	0.63	0.17	90,107,116,117	0
6	NAG	A	1325	14/15	0.69	0.23	63,79,86,88	14
6	NAG	A	1324	14/15	0.73	0.18	103,118,130,131	0
11	CO3	A	1337	4/4	0.80	0.18	73,77,78,81	0
11	CO3	A	1336	4/4	0.81	0.14	73,77,78,79	0
11	CO3	A	1335	4/4	0.86	0.10	55,70,75,76	0
10	SO4	A	1334	5/5	0.88	0.09	78,78,90,91	0
11	CO3	A	1338	4/4	0.89	0.13	34,39,43,48	4
9	CL	A	1329	1/1	0.96	0.09	29,29,29,29	1

*Continued on next page...*

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	SO4	A	1333	5/5	0.98	0.07	38,39,42,44	0
9	CL	A	1330	1/1	0.98	0.09	38,38,38,38	1
10	SO4	A	1332	5/5	0.98	0.05	44,44,47,50	0
9	CL	A	1331	1/1	0.99	0.05	36,36,36,36	1
8	NA	A	1328	1/1	0.99	0.04	24,24,24,24	1
5	HEM	A	1307	43/43	0.99	0.05	26,28,32,44	0
7	CA	A	1327	1/1	0.99	0.05	34,34,34,34	1
7	CA	A	1326	1/1	1.00	0.03	32,32,32,32	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.