



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 22, 2024 – 01:04 AM EDT

PDB ID : 3HDL  
Title : Crystal Structure of Highly Glycosylated Peroxidase from Royal Palm Tree  
Authors : Watanabe, L.; Moura, P.R.; Bleicher, L.; Nascimento, A.S.; Zamorano, L.S.; Calvete, J.J.; Bursakov, S.; Roig, M.G.; Shnyrov, V.L.; Polikarpov, I.  
Deposited on : 2009-05-07  
Resolution : 1.85 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](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	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

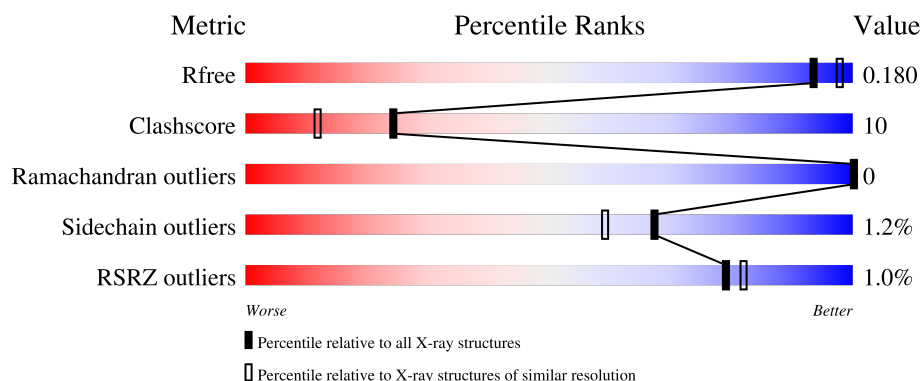
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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.




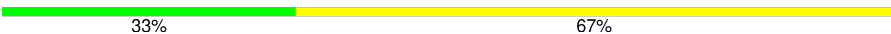
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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	304	<div> <div></div> <div>89%</div> <div>11%</div> </div>
2	B	7	<div> <div>86%</div> <div>14%</div> </div>
3	C	5	<div> <div>60%</div> <div>20%</div> <div>20%</div> </div>
4	D	3	<div> <div>67%</div> <div>33%</div> </div>
4	E	3	<div> <div>67%</div> <div>33%</div> </div>

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Mol	Chain	Length	Quality of chain
5	F	2	
6	G	6	

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
12	EDO	A	332	-	-	X	-
13	NAG	A	1200	X	-	-	-
3	MAN	C	3	X	-	-	-
5	NAG	F	2	X	-	-	-
6	MAN	G	5	X	-	-	-

## 2 Entry composition [i](#)

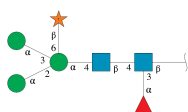
There are 14 unique types of molecules in this entry. The entry contains 3394 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Royal Palm Tree Peroxidase.

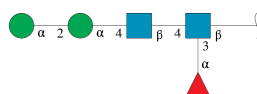
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	304	2288	1425	392	454	17	0	12	0

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)][beta-D-xylofuranose-(1-6)]alpha-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.



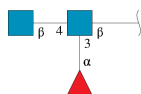
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	7	80	45	2	33	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-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	5	60	34	2	24	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.



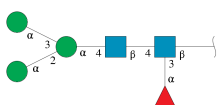
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			38	22	2	14			
4	E	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



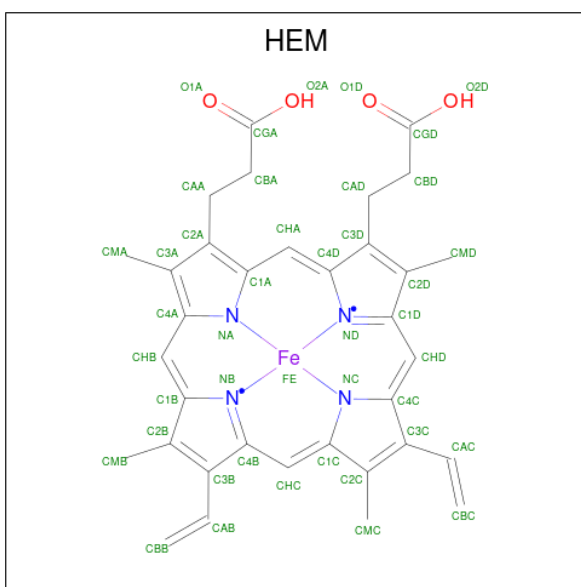
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]alpha-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
6	G	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 7 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>).

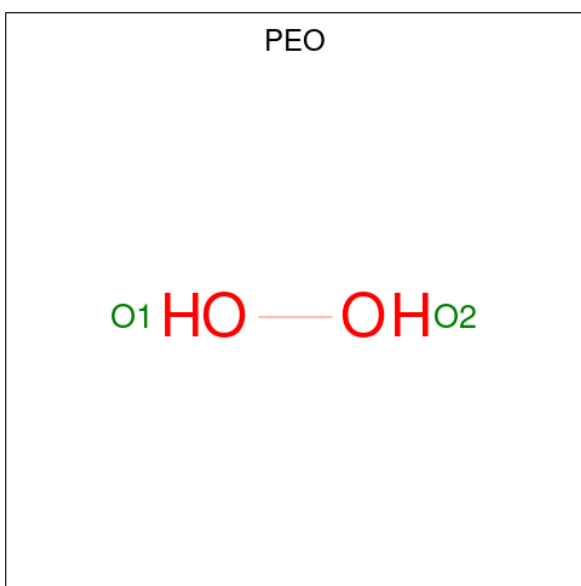


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

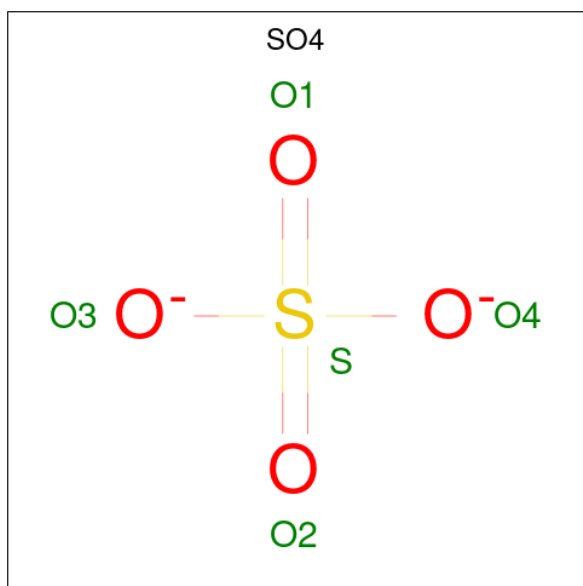
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total Ca 2 2	0	0

- Molecule 9 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula:  $\text{H}_2\text{O}_2$ ).



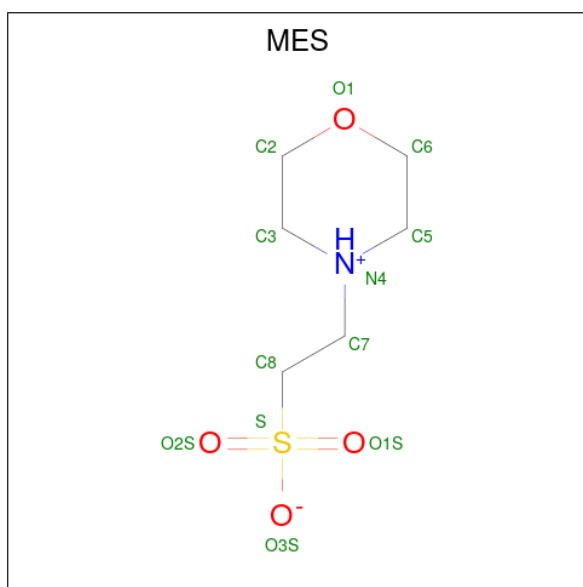
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O 2 2	0	0

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



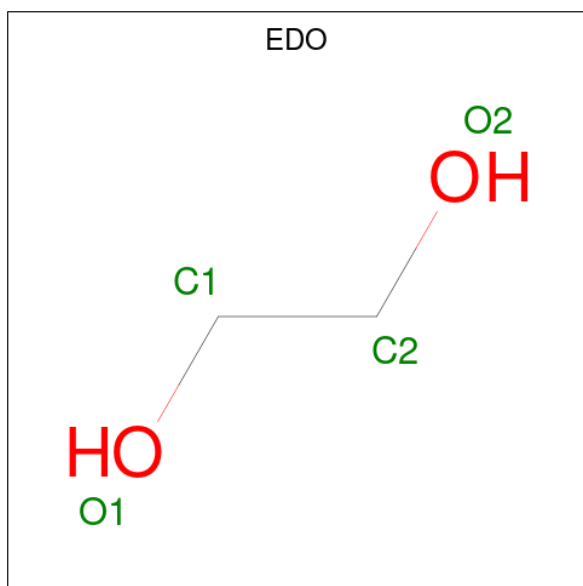
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total O S 5 4 1	0	0
10	A	1	Total O S 5 4 1	0	0
10	A	1	Total O S 5 4 1	0	0
10	A	1	Total O S 5 4 1	0	0
10	A	1	Total O S 5 4 1	0	0
10	A	1	Total O S 5 4 1	0	0
10	A	1	Total O S 5 4 1	0	0
10	A	1	Total O S 5 4 1	0	0

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 12 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			4	2	2		
12	A	1	Total	C	O	0	0
			4	2	2		
12	A	1	Total	C	O	0	0
			4	2	2		

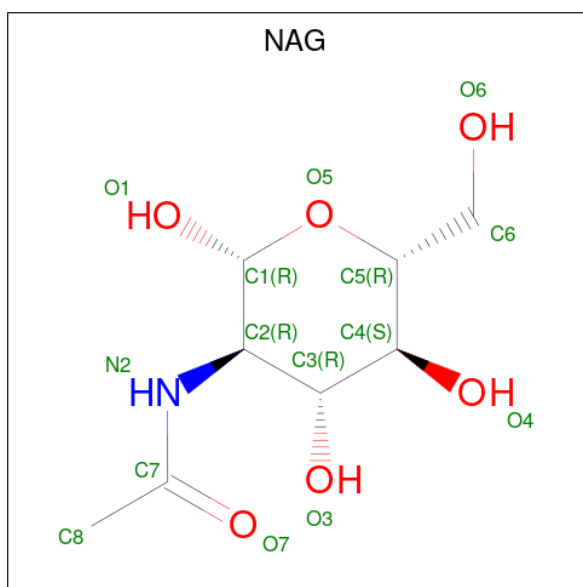
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			4	2	2		
12	A	1	Total	C	O	0	0
			4	2	2		
12	A	1	Total	C	O	0	0
			4	2	2		
12	A	1	Total	C	O	0	0
			4	2	2		
12	A	1	Total	C	O	0	0
			4	2	2		
12	A	1	Total	C	O	0	0
			4	2	2		
12	A	1	Total	C	O	0	0
			4	2	2		
12	A	1	Total	C	O	0	0
			4	2	2		
12	A	1	Total	C	O	0	0
			4	2	2		
12	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

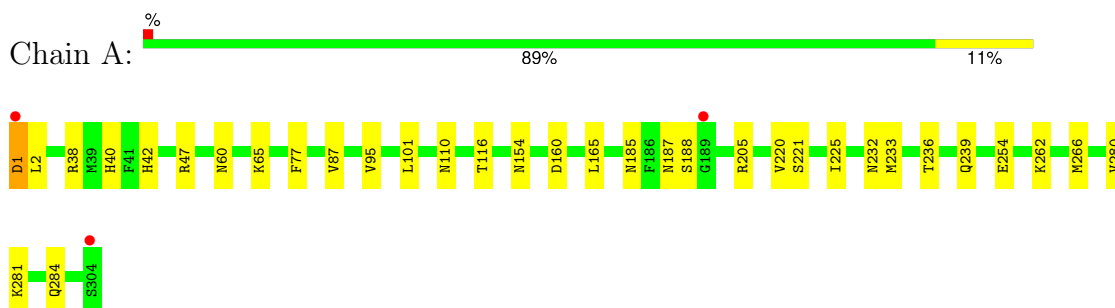
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	586	Total	O	0	0
			586	586		

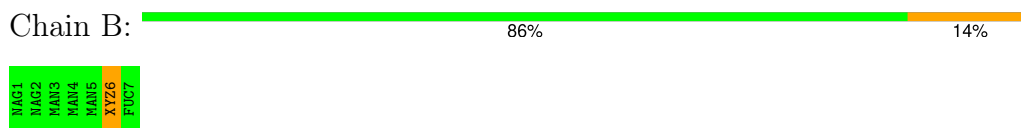
### 3 Residue-property plots

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

- Molecule 1: Royal Palm Tree Peroxidase



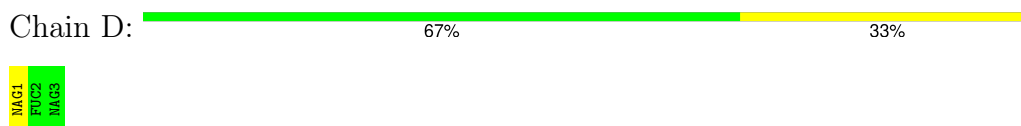
- Molecule 2: alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)][beta-D-xylofuranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-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

Chain E:  67% 33%

MAG1  
FUC2  
MAG3

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

Chain F:  50% 50%

MAG1  
MAG2

- Molecule 6: alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]alpha-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

Chain G:  33% 67%

MAG1  
MAG2  
MAN3  
MAN4  
MAN5  
FUC6

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.82Å 117.82Å 93.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.78 – 1.85 44.78 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.78-1.85) 99.8 (44.78-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 1.86Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.176 , 0.187 0.171 , 0.180	Depositor DCC
$R_{free}$ test set	3241 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.6	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 69.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3394	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: XYZ, EDO, MES, HEM, NAG, SO4, CA, FUC, MAN, PEO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/2357	0.44	0/3215

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	2288	0	2270	40	0
2	B	80	0	67	1	0
3	C	60	0	52	2	0
4	D	38	0	34	0	0
4	E	38	0	34	0	0
5	F	28	0	25	0	0
6	G	71	0	61	0	0
7	A	43	0	30	4	0
8	A	2	0	0	0	0
9	A	2	0	0	1	0
10	A	40	0	0	0	0
11	A	12	0	12	2	0
12	A	64	0	96	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	A	42	0	39	4	0
14	A	586	0	0	20	4
All	All	3394	0	2720	54	4

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 10.

The worst 5 of 54 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)
14:A:570:HOH:O	2:B:6:XYZ:H51	1.63	0.98
1:A:116:THR:OG1	14:A:367:HOH:O	1.90	0.88
1:A:47:ARG:HH12	12:A:326:EDO:H21	1.38	0.88
1:A:232:ASN:HD21	12:A:322:EDO:H12	1.40	0.87
13:A:1100:NAG:H2	14:A:554:HOH:O	1.80	0.82

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:575:HOH:O	14:A:580:HOH:O[3_564]	1.71	0.49
14:A:518:HOH:O	14:A:582:HOH:O[6_555]	1.81	0.39
14:A:913:HOH:O	14:A:915:HOH:O[2_665]	1.89	0.31
14:A:488:HOH:O	14:A:492:HOH:O[3_564]	2.13	0.07

## 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	314/304 (103%)	311 (99%)	3 (1%)	0	<a href="#">100</a> <a href="#">100</a>

There are no Ramachandran outliers to report.

### 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	256/244 (105%)	252 (98%)	4 (2%)	58 46

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

Mol	Chain	Res	Type
1	A	1	ASP
1	A	101[A]	LEU
1	A	101[B]	LEU
1	A	110	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	110	ASN
1	A	118	GLN
1	A	137	GLN
1	A	187	ASN

### 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

26 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	0.51	0	17,19,21	0.70	0
2	NAG	B	2	2	14,14,15	0.47	0	17,19,21	0.72	0
2	MAN	B	3	2	11,11,12	0.69	0	15,15,17	0.50	0
2	MAN	B	4	2	11,11,12	0.56	0	15,15,17	0.60	0
2	MAN	B	5	2	11,11,12	0.62	0	15,15,17	0.77	0
2	XYZ	B	6	2	9,9,10	0.43	0	11,12,14	1.56	2 (18%)
2	FUC	B	7	2	10,10,11	0.67	0	14,14,16	0.52	0
3	NAG	C	1	1,3	14,14,15	0.44	0	17,19,21	1.01	1 (5%)
3	NAG	C	2	3	14,14,15	0.48	0	17,19,21	0.75	0
3	MAN	C	3	3	11,11,12	0.60	0	15,15,17	0.45	0
3	MAN	C	4	3	11,11,12	0.62	0	15,15,17	1.18	2 (13%)
3	FUC	C	5	3	10,10,11	0.64	0	14,14,16	0.48	0
4	NAG	D	1	1,4	14,14,15	0.47	0	17,19,21	1.09	1 (5%)
4	FUC	D	2	4	10,10,11	0.66	0	14,14,16	0.64	0
4	NAG	D	3	4	14,14,15	0.49	0	17,19,21	0.75	0
4	NAG	E	1	1,4	14,14,15	0.53	0	17,19,21	0.58	0
4	FUC	E	2	4	10,10,11	0.64	0	14,14,16	0.59	0
4	NAG	E	3	4	14,14,15	0.46	0	17,19,21	0.85	1 (5%)
5	NAG	F	1	1,5	14,14,15	0.52	0	17,19,21	0.62	0
5	NAG	F	2	5	14,14,15	0.46	0	17,19,21	0.75	1 (5%)
6	NAG	G	1	1,6	14,14,15	0.47	0	17,19,21	0.89	1 (5%)
6	NAG	G	2	6	14,14,15	0.48	0	17,19,21	0.80	1 (5%)
6	MAN	G	3	6	11,11,12	0.73	0	15,15,17	1.27	3 (20%)
6	MAN	G	4	6	11,11,12	0.57	0	15,15,17	0.56	0
6	MAN	G	5	6	11,11,12	0.66	0	15,15,17	1.12	1 (6%)
6	FUC	G	6	6	10,10,11	0.68	0	14,14,16	0.59	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	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	MAN	B	3	2	-	1/2/19/22	0/1/1/1
2	MAN	B	4	2	-	1/2/19/22	1/1/1/1
2	MAN	B	5	2	-	2/2/19/22	0/1/1/1
2	XYZ	B	6	2	-	0/2/15/18	0/1/1/1
2	FUC	B	7	2	-	-	0/1/1/1
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	MAN	C	3	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
3	FUC	C	5	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	-	3/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	FUC	E	2	4	-	-	0/1/1/1
4	NAG	E	3	4	-	0/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	G	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	MAN	G	3	6	-	1/2/19/22	0/1/1/1
6	MAN	G	4	6	-	1/2/19/22	1/1/1/1
6	MAN	G	5	6	1/1/4/5	2/2/19/22	0/1/1/1
6	FUC	G	6	6	-	-	0/1/1/1

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6	XYZ	O4-C4-C3	3.52	107.89	104.63
6	G	5	MAN	C3-C4-C5	3.39	116.38	110.23
3	C	1	NAG	C1-O5-C5	3.16	116.42	112.19
4	D	1	NAG	C1-O5-C5	2.77	115.89	112.19
2	B	6	XYZ	C1-C2-C3	2.75	106.03	101.63

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	3	MAN	C1
5	F	2	NAG	C1
6	G	5	MAN	C1

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
4	D	3	NAG	C8-C7-N2-C2
4	D	3	NAG	O7-C7-N2-C2
5	F	2	NAG	C1-C2-N2-C7

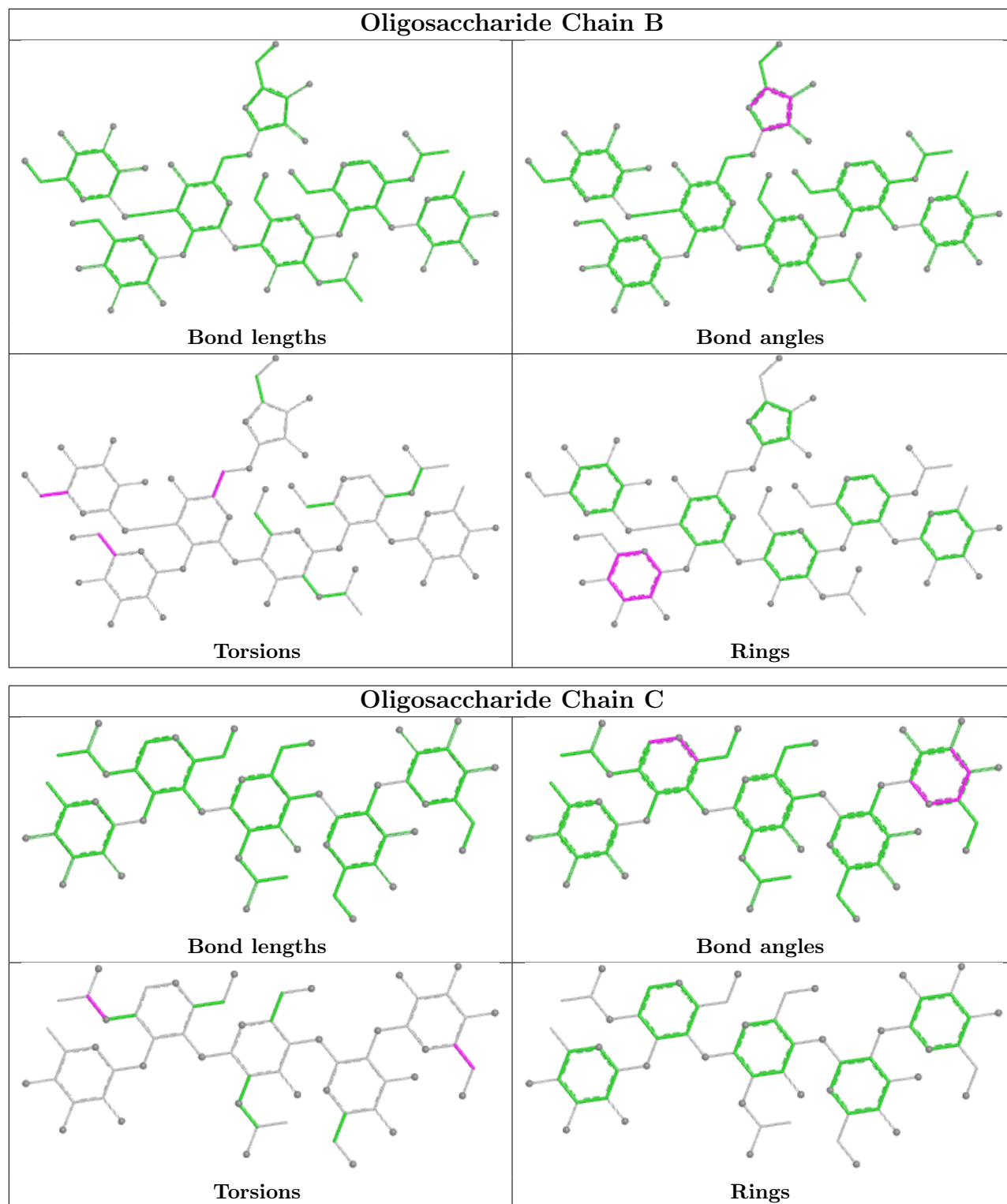
All (2) ring outliers are listed below:

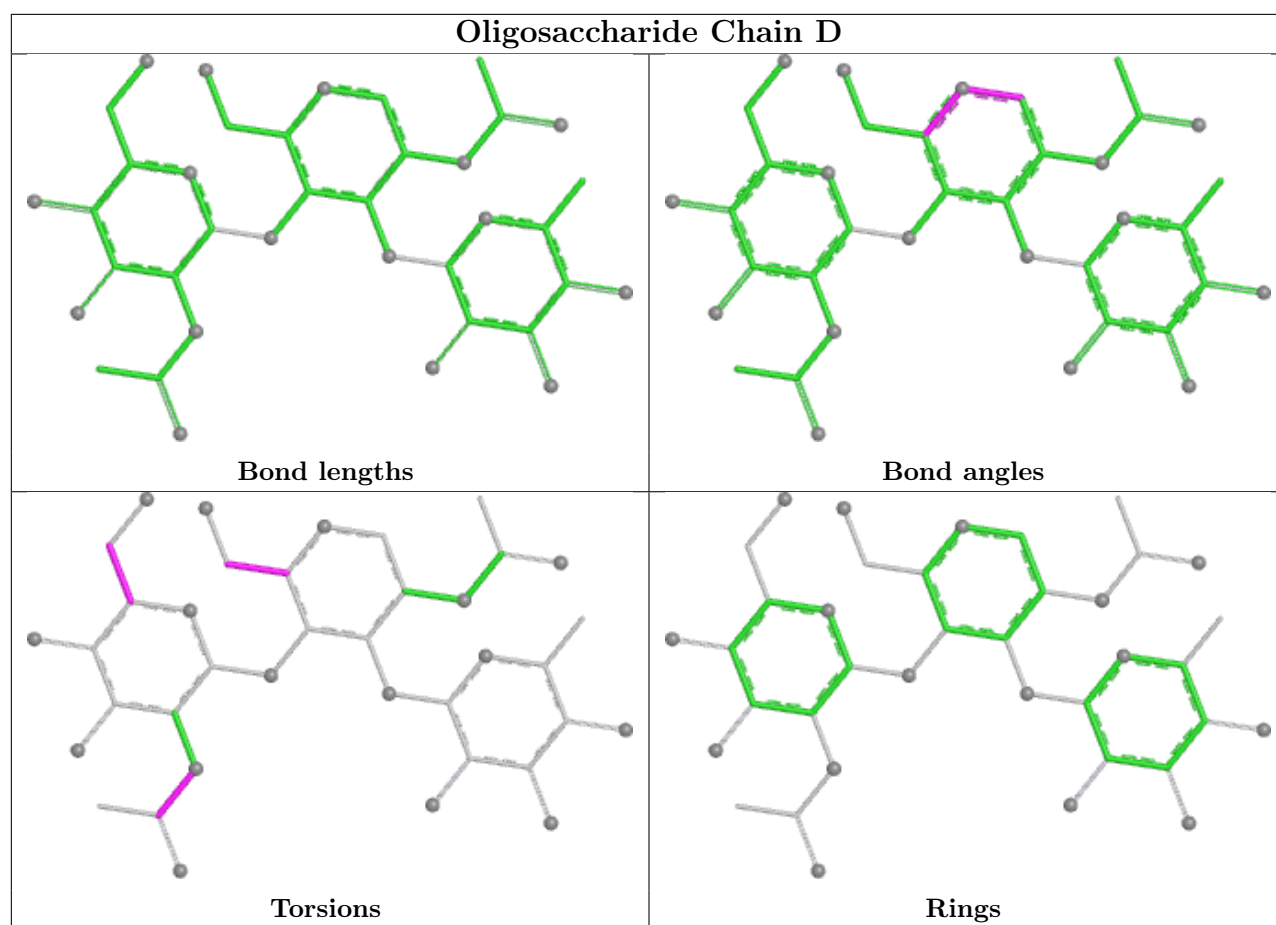
Mol	Chain	Res	Type	Atoms
2	B	4	MAN	C1-C2-C3-C4-C5-O5
6	G	4	MAN	C1-C2-C3-C4-C5-O5

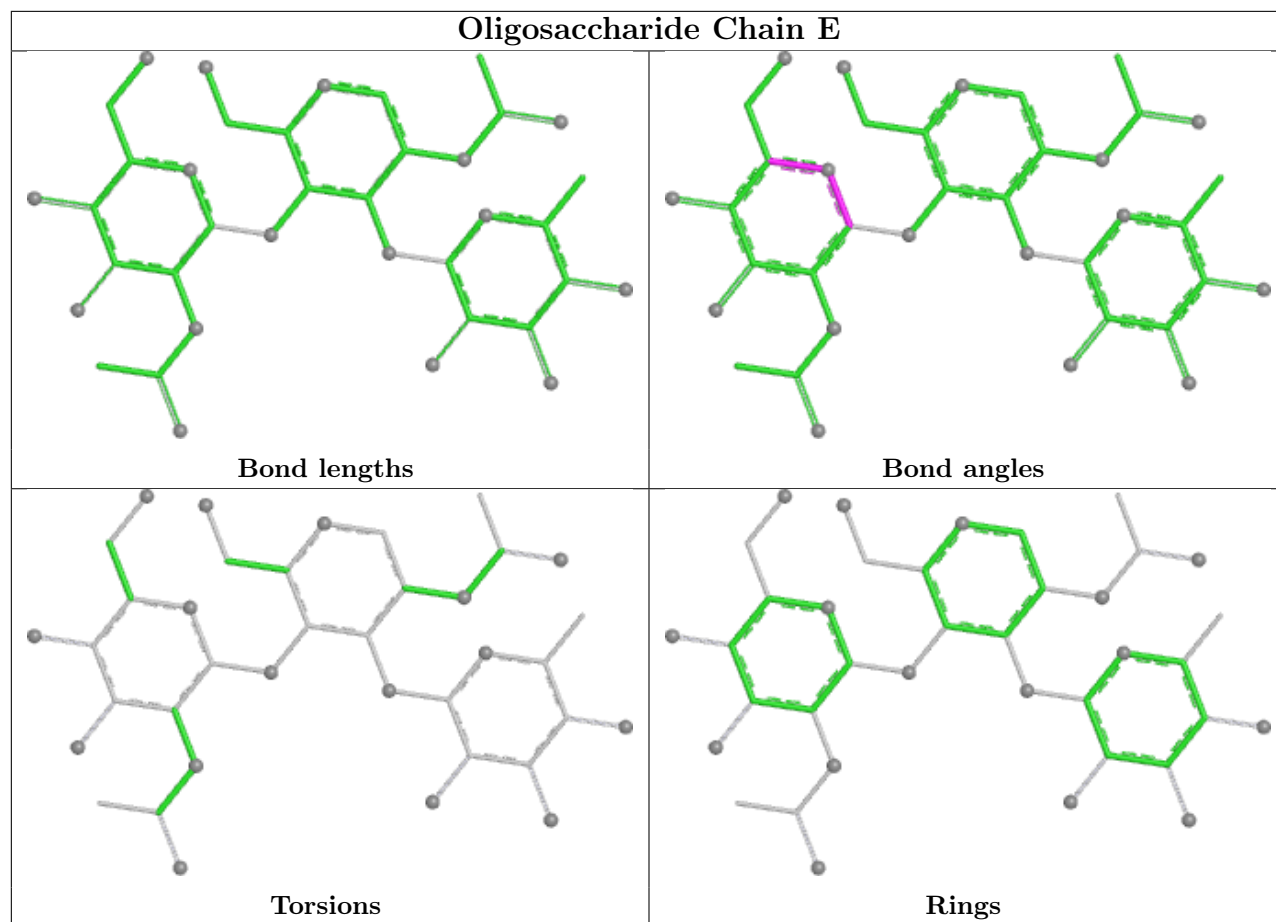
2 monomers are involved in 3 short contacts:

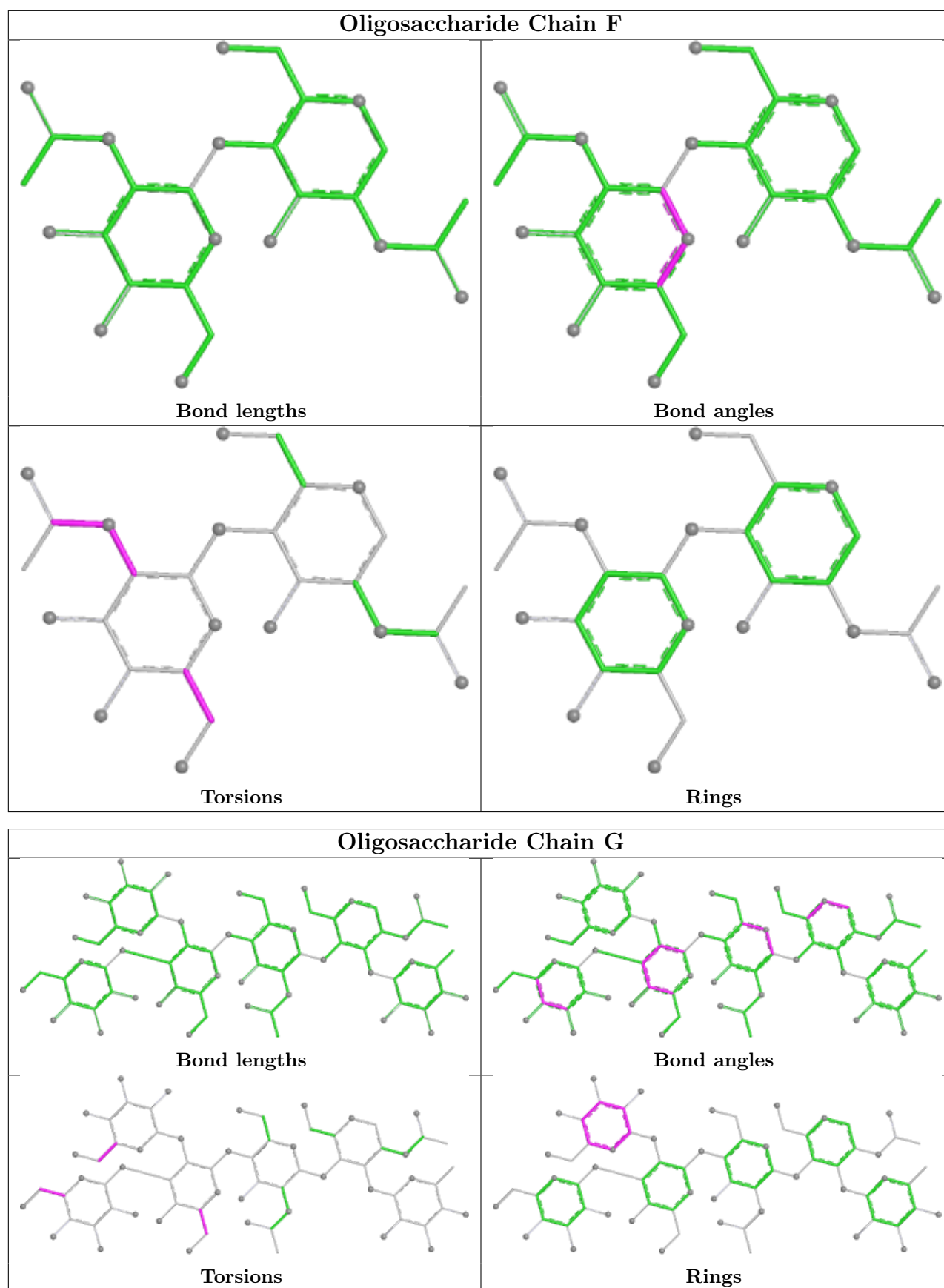
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	4	MAN	2	0
2	B	6	XYZ	1	0

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

Of 32 ligands modelled in this entry, 2 are monoatomic - leaving 30 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
13	NAG	A	700	1	14,14,15	0.47	0	17,19,21	1.04	3 (17%)
10	SO4	A	316	-	4,4,4	0.25	0	6,6,6	0.06	0
12	EDO	A	324	-	3,3,3	0.42	0	2,2,2	0.46	0
10	SO4	A	318	-	4,4,4	0.24	0	6,6,6	0.08	0
10	SO4	A	312	-	4,4,4	0.21	0	6,6,6	0.10	0
10	SO4	A	311	-	4,4,4	0.25	0	6,6,6	0.11	0
12	EDO	A	329	-	3,3,3	0.41	0	2,2,2	0.46	0
12	EDO	A	327	-	3,3,3	0.41	0	2,2,2	0.47	0
10	SO4	A	313	-	4,4,4	0.24	0	6,6,6	0.09	0
12	EDO	A	323	-	3,3,3	0.43	0	2,2,2	0.43	0
10	SO4	A	314	-	4,4,4	0.23	0	6,6,6	0.15	0
12	EDO	A	333	-	3,3,3	0.47	0	2,2,2	0.29	0
7	HEM	A	305	1,9	42,50,50	1.90	7 (16%)	46,82,82	1.72	8 (17%)
12	EDO	A	331	-	3,3,3	0.45	0	2,2,2	0.33	0
12	EDO	A	330	-	3,3,3	0.44	0	2,2,2	0.35	0
12	EDO	A	328	-	3,3,3	0.43	0	2,2,2	0.41	0
12	EDO	A	322	-	3,3,3	0.42	0	2,2,2	0.37	0
10	SO4	A	315	-	4,4,4	0.23	0	6,6,6	0.14	0
12	EDO	A	326	-	3,3,3	0.43	0	2,2,2	0.38	0
12	EDO	A	336	-	3,3,3	0.41	0	2,2,2	0.36	0
12	EDO	A	332	-	3,3,3	0.39	0	2,2,2	0.45	0
9	PEO	A	309	7	1,1,1	0.08	0	-		
12	EDO	A	320	-	3,3,3	0.27	0	2,2,2	0.87	0
11	MES	A	319	-	12,12,12	2.18	1 (8%)	15,16,16	2.37	6 (40%)
13	NAG	A	1200	1	14,14,15	0.52	0	17,19,21	0.73	0
12	EDO	A	335	-	3,3,3	0.43	0	2,2,2	0.37	0
12	EDO	A	321	-	3,3,3	0.36	0	2,2,2	0.48	0
12	EDO	A	334	-	3,3,3	0.43	0	2,2,2	0.35	0
13	NAG	A	1100	1	14,14,15	0.46	0	17,19,21	1.53	4 (23%)
10	SO4	A	317	-	4,4,4	0.23	0	6,6,6	0.14	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
13	NAG	A	700	1	-	3/6/23/26	0/1/1/1
12	EDO	A	324	-	-	1/1/1/1	-
12	EDO	A	329	-	-	0/1/1/1	-
12	EDO	A	327	-	-	0/1/1/1	-
12	EDO	A	333	-	-	0/1/1/1	-
12	EDO	A	323	-	-	1/1/1/1	-
7	HEM	A	305	1,9	-	4/12/54/54	-
12	EDO	A	331	-	-	0/1/1/1	-
12	EDO	A	330	-	-	0/1/1/1	-
12	EDO	A	328	-	-	0/1/1/1	-
12	EDO	A	322	-	-	1/1/1/1	-
12	EDO	A	326	-	-	0/1/1/1	-
12	EDO	A	336	-	-	0/1/1/1	-
12	EDO	A	332	-	-	1/1/1/1	-
12	EDO	A	320	-	-	0/1/1/1	-
13	NAG	A	1200	1	1/1/5/7	5/6/23/26	0/1/1/1
11	MES	A	319	-	-	5/6/14/14	0/1/1/1
12	EDO	A	335	-	-	0/1/1/1	-
12	EDO	A	321	-	-	0/1/1/1	-
12	EDO	A	334	-	-	0/1/1/1	-
13	NAG	A	1100	1	-	3/6/23/26	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	305	HEM	C3D-C2D	7.57	1.53	1.36
11	A	319	MES	C8-S	-7.31	1.67	1.77
7	A	305	HEM	C3C-C2C	-4.20	1.34	1.40
7	A	305	HEM	C3C-CAC	3.49	1.55	1.47
7	A	305	HEM	CAB-C3B	2.83	1.54	1.47

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	319	MES	C5-N4-C3	5.83	121.39	108.84
7	A	305	HEM	C4D-ND-C1D	5.35	111.54	105.21
13	A	1100	NAG	C1-O5-C5	4.06	117.62	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
7	A	305	HEM	CBD-CAD-C3D	-3.85	101.89	112.53
11	A	319	MES	C7-N4-C3	3.40	120.30	111.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	1200	NAG	C1

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	319	MES	C7-C8-S-O2S
11	A	319	MES	C7-C8-S-O3S
13	A	700	NAG	C1-C2-N2-C7
13	A	700	NAG	C8-C7-N2-C2
13	A	700	NAG	O7-C7-N2-C2

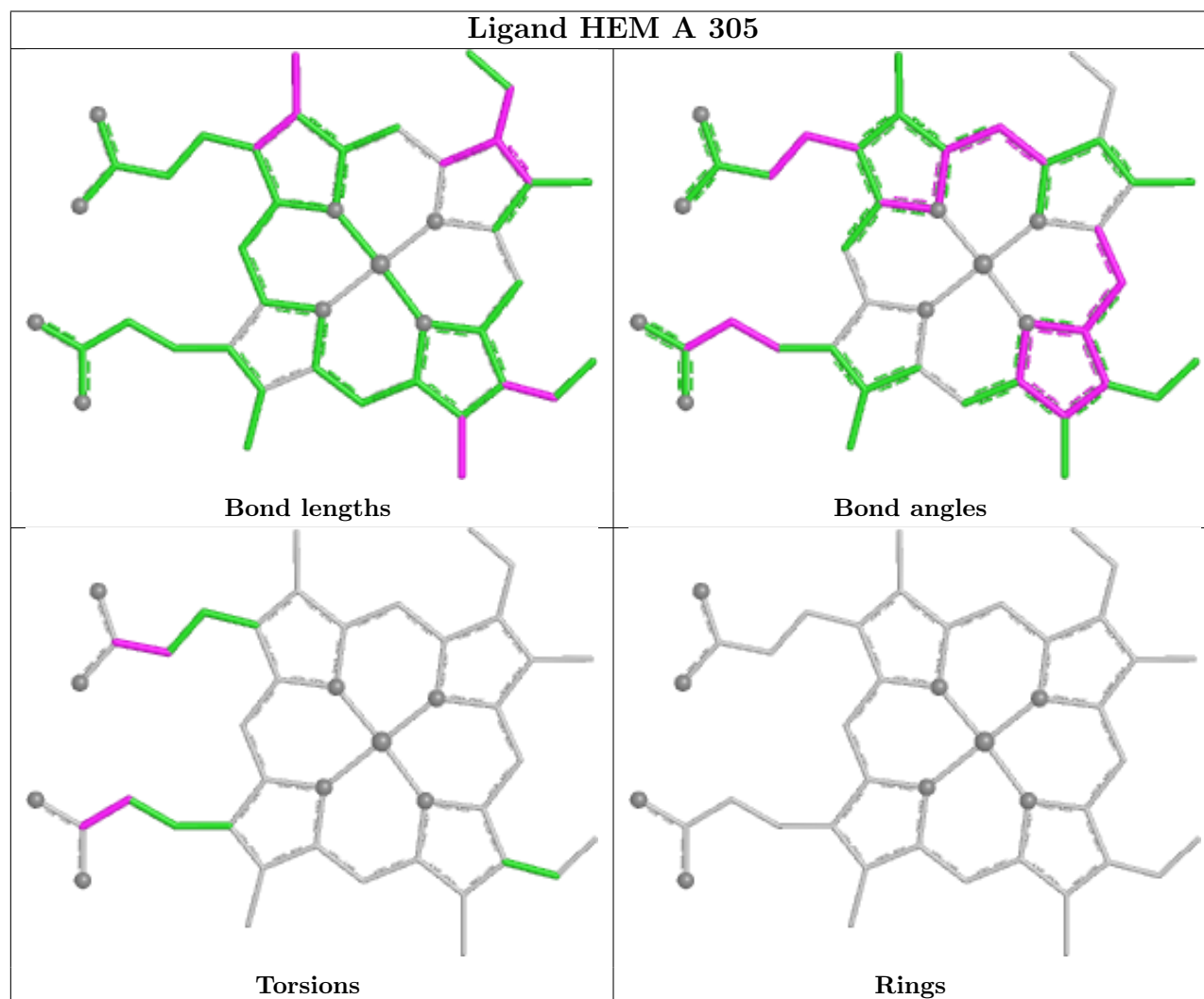
There are no ring outliers.

16 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	700	NAG	1	0
12	A	324	EDO	2	0
12	A	327	EDO	1	0
12	A	323	EDO	1	0
7	A	305	HEM	4	0
12	A	330	EDO	2	0
12	A	322	EDO	1	0
12	A	326	EDO	2	0
12	A	336	EDO	2	0
12	A	332	EDO	4	0
9	A	309	PEO	1	0
12	A	320	EDO	2	0
11	A	319	MES	2	0
12	A	335	EDO	1	0
12	A	321	EDO	3	0
13	A	1100	NAG	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	304/304 (100%)	-0.39	3 (0%) 79 82	12, 28, 42, 63	14 (4%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	304	SER	4.7
1	A	189	GLY	2.7
1	A	1	ASP	2.1

### 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
6	MAN	G	5	11/12	0.56	0.16	109,111,115,116	0
2	MAN	B	5	11/12	0.62	0.16	103,109,116,117	0
4	NAG	E	3	14/15	0.63	0.17	102,108,117,120	0
5	NAG	F	2	14/15	0.68	0.18	91,96,102,103	0
2	MAN	B	4	11/12	0.71	0.23	78,98,108,108	0
2	XYZ	B	6	9/10	0.73	0.18	94,98,103,108	0
4	NAG	D	3	14/15	0.77	0.16	75,80,87,92	0
3	MAN	C	3	11/12	0.77	0.15	68,78,88,89	0
3	FUC	C	5	10/11	0.78	0.18	74,83,86,94	0

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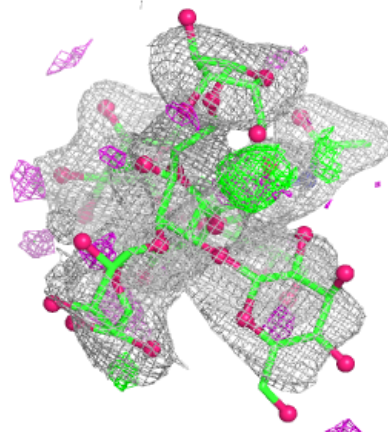
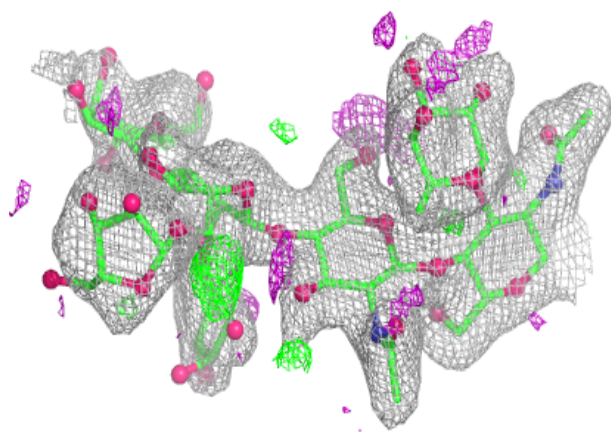
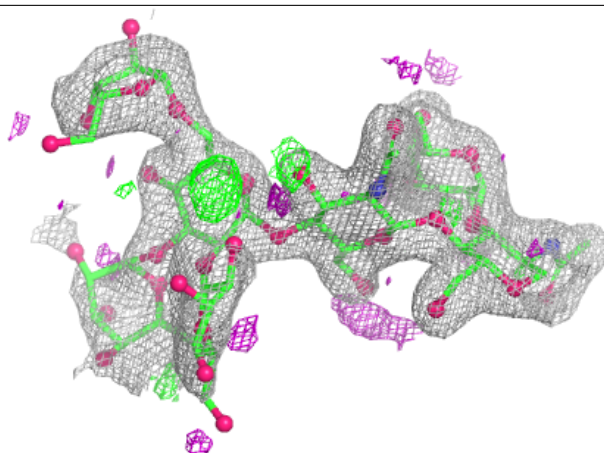
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	F	1	14/15	0.78	0.16	54,65,76,80	0
2	MAN	B	3	11/12	0.78	0.14	59,82,94,99	0
6	MAN	G	3	11/12	0.78	0.15	85,101,107,109	0
6	MAN	G	4	11/12	0.78	0.15	72,84,95,105	0
4	FUC	E	2	10/11	0.78	0.16	89,94,99,101	0
3	MAN	C	4	11/12	0.82	0.18	54,66,92,97	0
4	FUC	D	2	10/11	0.82	0.17	62,79,83,85	0
4	NAG	D	1	14/15	0.85	0.14	37,60,71,73	0
4	NAG	E	1	14/15	0.86	0.13	49,70,85,86	0
6	NAG	G	2	14/15	0.87	0.12	44,51,65,66	0
3	NAG	C	2	14/15	0.88	0.12	51,60,69,85	0
3	NAG	C	1	14/15	0.88	0.13	52,59,74,91	0
6	FUC	G	6	10/11	0.89	0.13	49,58,63,65	0
2	NAG	B	2	14/15	0.92	0.10	37,46,53,57	0
6	NAG	G	1	14/15	0.94	0.09	33,38,48,53	0
2	FUC	B	7	10/11	0.94	0.10	34,47,49,57	0
2	NAG	B	1	14/15	0.95	0.10	30,37,47,48	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.

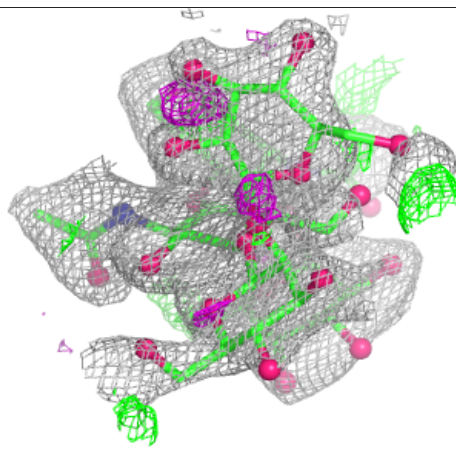
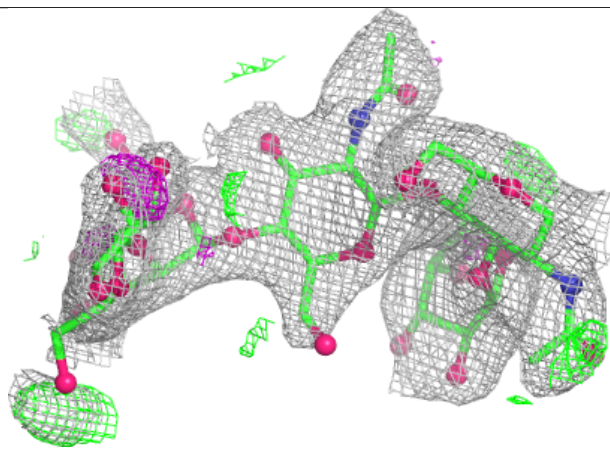
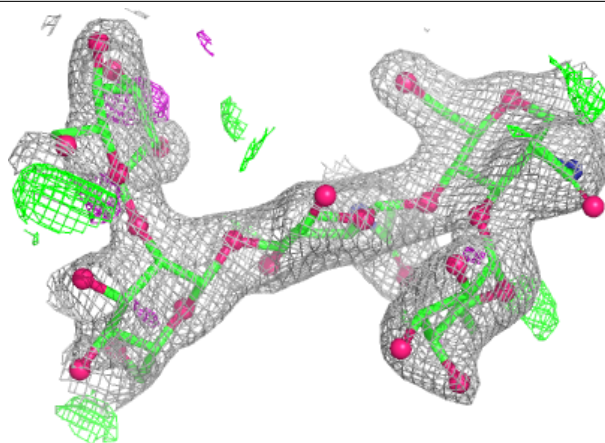
**Electron density around Chain B:**

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



**Electron density around Chain C:**

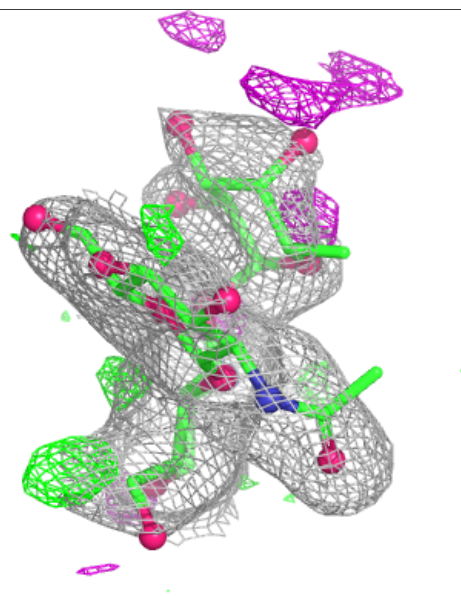
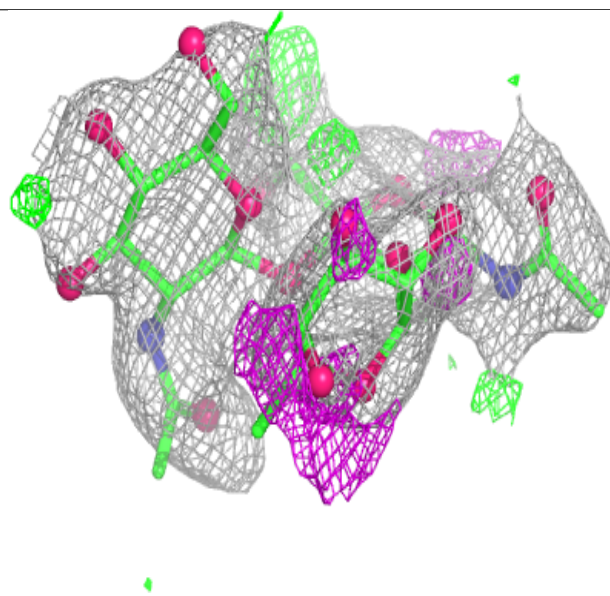
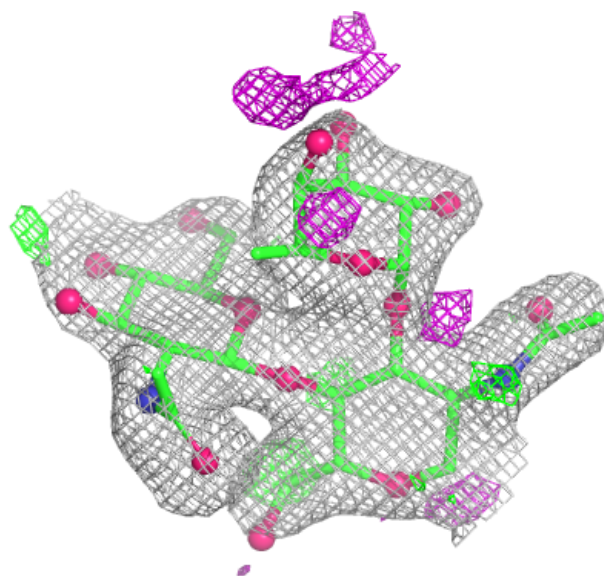
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around Chain D:**

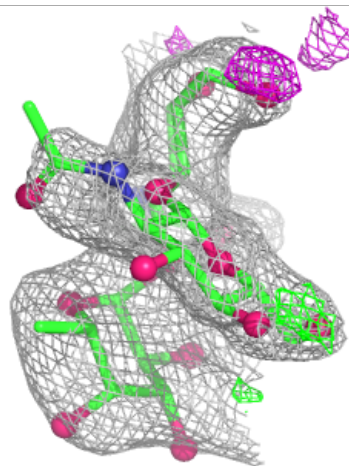
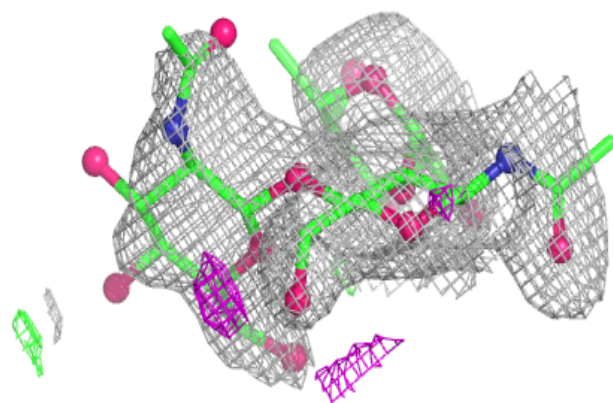
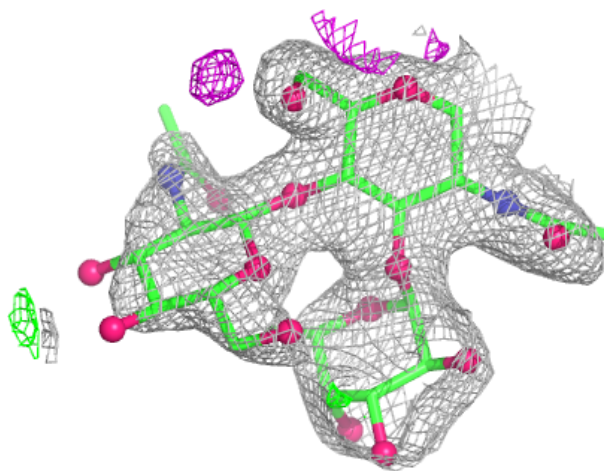
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





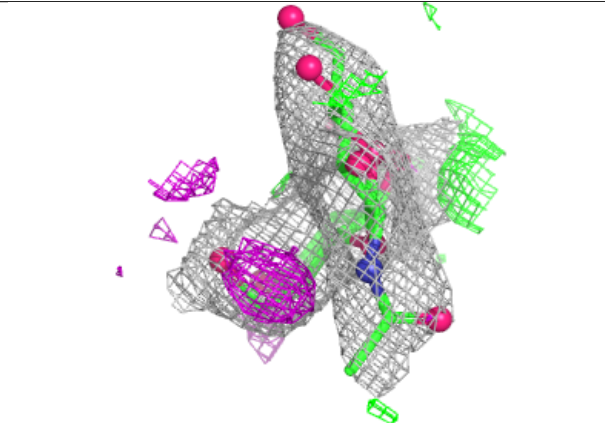
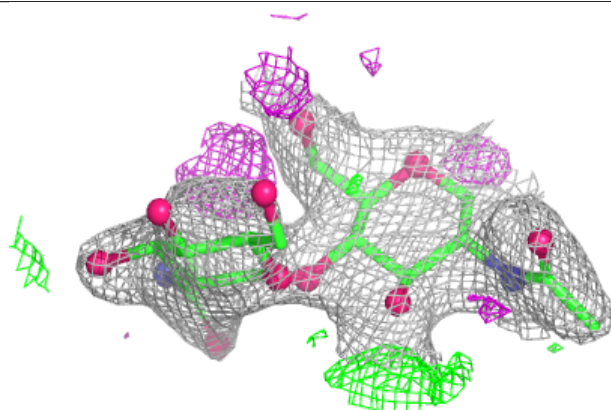
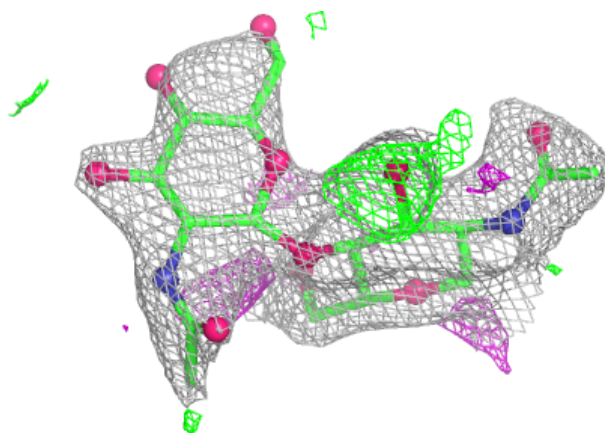
**Electron density around Chain E:**

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

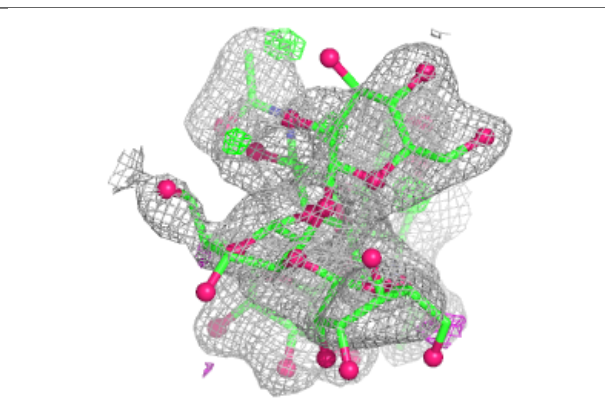
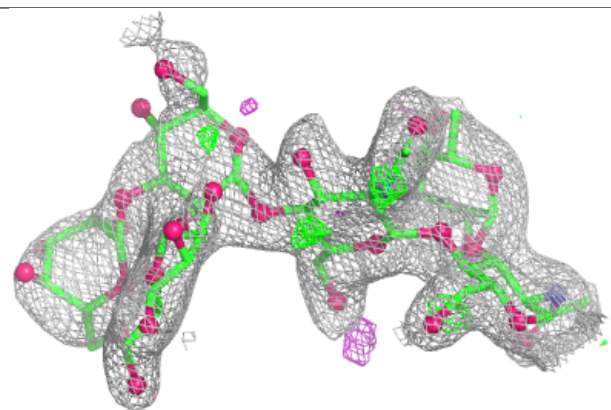
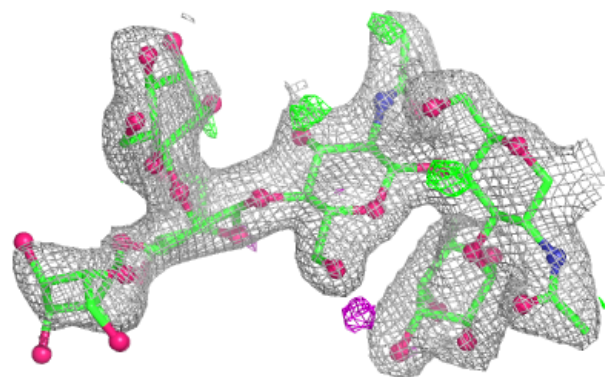


**Electron density around Chain F:**

$2mF_o-DF_c$  (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)

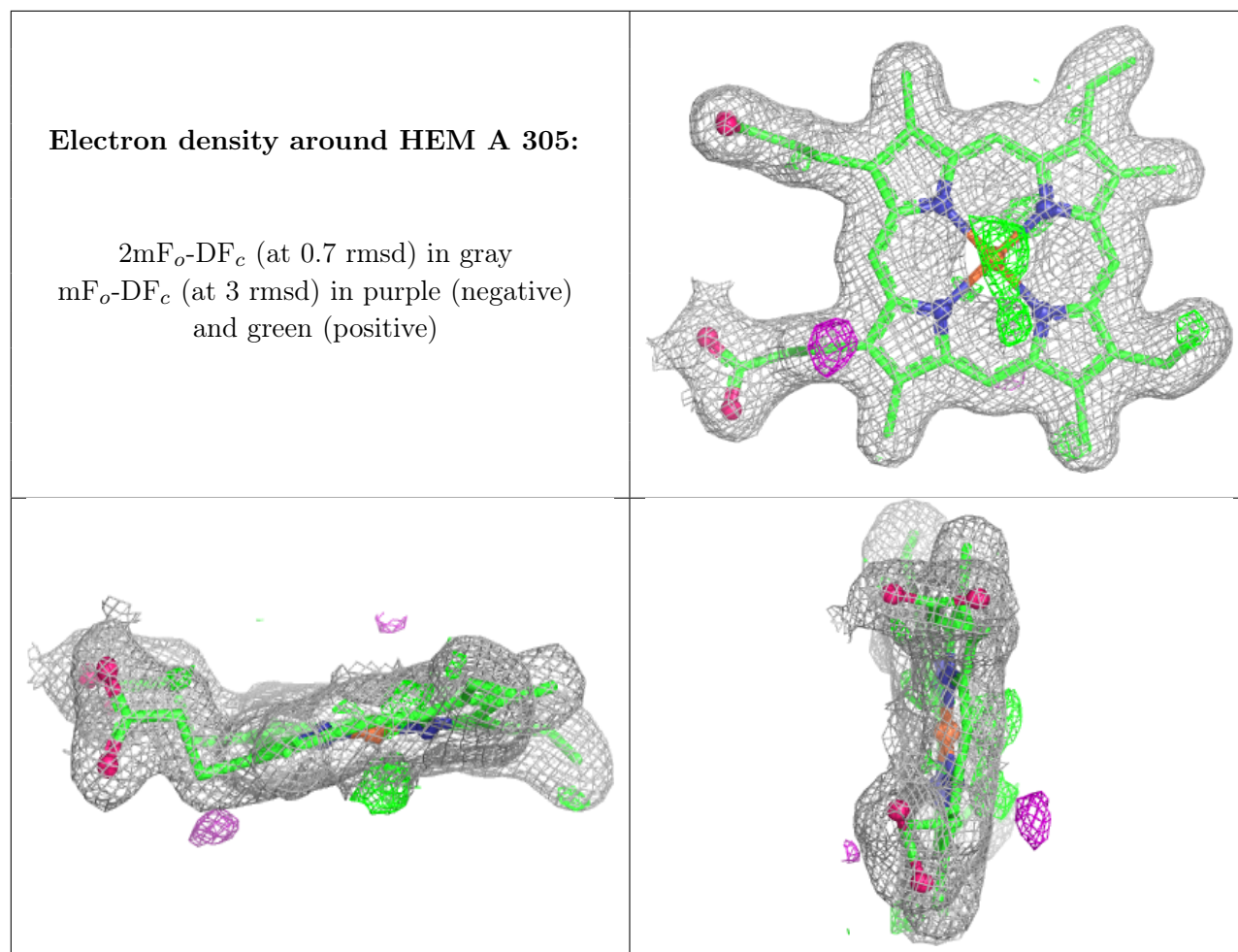


## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
13	NAG	A	1100	14/15	0.47	0.24	81,102,111,119	0
12	EDO	A	323	4/4	0.54	0.27	78,83,84,86	0
10	SO4	A	311	5/5	0.67	0.21	116,117,118,123	0
13	NAG	A	1200	14/15	0.68	0.22	91,108,116,124	0
10	SO4	A	317	5/5	0.73	0.14	116,120,122,126	0
10	SO4	A	316	5/5	0.76	0.16	96,106,109,112	0
13	NAG	A	700	14/15	0.76	0.18	64,95,107,110	0
12	EDO	A	324	4/4	0.78	0.23	52,57,57,58	0
12	EDO	A	330	4/4	0.79	0.23	45,66,71,73	0
10	SO4	A	318	5/5	0.80	0.13	113,114,116,117	0
12	EDO	A	335	4/4	0.85	0.21	37,45,54,60	0
12	EDO	A	326	4/4	0.86	0.17	59,67,71,73	0
12	EDO	A	322	4/4	0.87	0.16	45,47,50,67	0
12	EDO	A	332	4/4	0.87	0.15	55,57,66,66	0
12	EDO	A	327	4/4	0.87	0.27	62,63,67,68	0
12	EDO	A	334	4/4	0.88	0.17	45,52,55,67	0
10	SO4	A	313	5/5	0.89	0.13	74,87,96,102	0
12	EDO	A	336	4/4	0.90	0.13	38,50,57,60	0
12	EDO	A	320	4/4	0.91	0.22	30,32,34,49	0
12	EDO	A	321	4/4	0.92	0.25	35,43,46,54	0
12	EDO	A	329	4/4	0.92	0.17	49,51,62,65	0
12	EDO	A	333	4/4	0.93	0.14	29,40,48,49	0
10	SO4	A	315	5/5	0.94	0.10	51,55,60,81	0
12	EDO	A	328	4/4	0.94	0.12	37,41,53,65	0
10	SO4	A	314	5/5	0.95	0.09	30,42,49,65	0
11	MES	A	319	12/12	0.96	0.10	33,36,46,48	0
9	PEO	A	309	2/2	0.97	0.09	27,27,27,31	1
10	SO4	A	312	5/5	0.98	0.10	34,40,44,53	0
12	EDO	A	331	4/4	0.98	0.10	30,37,43,49	0
8	CA	A	307	1/1	0.99	0.04	27,27,27,27	0
7	HEM	A	305	43/43	0.99	0.05	18,23,26,29	0
8	CA	A	306	1/1	1.00	0.03	25,25,25,25	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.