



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 29, 2025 – 08:42 am BST

PDB ID : 9FHY / pdb\_00009fhy  
Title : Bacteroides ovatus polysaccharide lyase family 38 (BoPL38) wild type in complex with an unsaturated mannuronic acid tetramer at pH 3.5  
Authors : Tandrup, T.; Wilkens, C.  
Deposited on : 2024-05-28  
Resolution : 1.76 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 Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
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)	:	2.44

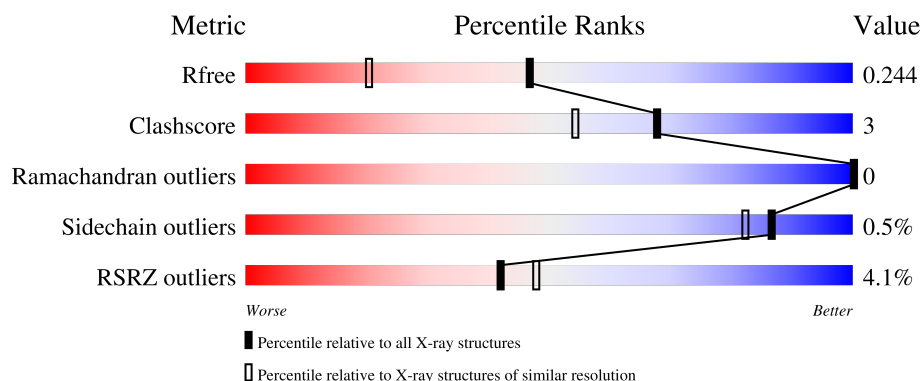
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.76 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.



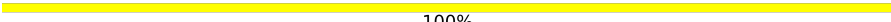
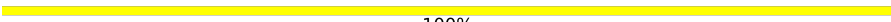

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (1.76-1.76)

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	404	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>6%</div> </div> </div>
1	B	404	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>6%</div> </div> </div>
1	C	404	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>6%</div> </div> </div>
1	D	404	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>6%</div> </div> </div>
2	E	3	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	3	 100%
2	G	3	 100%
2	H	3	 100%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13124 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 Alginate lyase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	2	0
			3066	1961	519	573	13			
1	B	380	Total	C	N	O	S	0	2	0
			3064	1961	519	571	13			
1	C	380	Total	C	N	O	S	0	0	0
			3052	1952	516	571	13			
1	D	380	Total	C	N	O	S	0	0	0
			3052	1952	516	571	13			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A5M5BWR5
A	2	GLY	-	expression tag	UNP A0A5M5BWR5
A	3	SER	-	expression tag	UNP A0A5M5BWR5
A	4	SER	-	expression tag	UNP A0A5M5BWR5
A	5	HIS	-	expression tag	UNP A0A5M5BWR5
A	6	HIS	-	expression tag	UNP A0A5M5BWR5
A	7	HIS	-	expression tag	UNP A0A5M5BWR5
A	8	HIS	-	expression tag	UNP A0A5M5BWR5
A	9	HIS	-	expression tag	UNP A0A5M5BWR5
A	10	HIS	-	expression tag	UNP A0A5M5BWR5
A	11	SER	-	expression tag	UNP A0A5M5BWR5
A	12	SER	-	expression tag	UNP A0A5M5BWR5
A	13	GLY	-	expression tag	UNP A0A5M5BWR5
A	14	LEU	-	expression tag	UNP A0A5M5BWR5
A	15	VAL	-	expression tag	UNP A0A5M5BWR5
A	16	PRO	-	expression tag	UNP A0A5M5BWR5
A	17	ARG	-	expression tag	UNP A0A5M5BWR5
A	18	GLY	-	expression tag	UNP A0A5M5BWR5
A	19	SER	-	expression tag	UNP A0A5M5BWR5
A	20	HIS	-	expression tag	UNP A0A5M5BWR5
A	21	MET	-	expression tag	UNP A0A5M5BWR5

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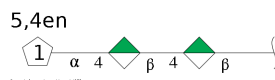
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	-	expression tag	UNP A0A5M5BWR5
A	23	SER	-	expression tag	UNP A0A5M5BWR5
B	1	MET	-	initiating methionine	UNP A0A5M5BWR5
B	2	GLY	-	expression tag	UNP A0A5M5BWR5
B	3	SER	-	expression tag	UNP A0A5M5BWR5
B	4	SER	-	expression tag	UNP A0A5M5BWR5
B	5	HIS	-	expression tag	UNP A0A5M5BWR5
B	6	HIS	-	expression tag	UNP A0A5M5BWR5
B	7	HIS	-	expression tag	UNP A0A5M5BWR5
B	8	HIS	-	expression tag	UNP A0A5M5BWR5
B	9	HIS	-	expression tag	UNP A0A5M5BWR5
B	10	HIS	-	expression tag	UNP A0A5M5BWR5
B	11	SER	-	expression tag	UNP A0A5M5BWR5
B	12	SER	-	expression tag	UNP A0A5M5BWR5
B	13	GLY	-	expression tag	UNP A0A5M5BWR5
B	14	LEU	-	expression tag	UNP A0A5M5BWR5
B	15	VAL	-	expression tag	UNP A0A5M5BWR5
B	16	PRO	-	expression tag	UNP A0A5M5BWR5
B	17	ARG	-	expression tag	UNP A0A5M5BWR5
B	18	GLY	-	expression tag	UNP A0A5M5BWR5
B	19	SER	-	expression tag	UNP A0A5M5BWR5
B	20	HIS	-	expression tag	UNP A0A5M5BWR5
B	21	MET	-	expression tag	UNP A0A5M5BWR5
B	22	ALA	-	expression tag	UNP A0A5M5BWR5
B	23	SER	-	expression tag	UNP A0A5M5BWR5
C	1	MET	-	initiating methionine	UNP A0A5M5BWR5
C	2	GLY	-	expression tag	UNP A0A5M5BWR5
C	3	SER	-	expression tag	UNP A0A5M5BWR5
C	4	SER	-	expression tag	UNP A0A5M5BWR5
C	5	HIS	-	expression tag	UNP A0A5M5BWR5
C	6	HIS	-	expression tag	UNP A0A5M5BWR5
C	7	HIS	-	expression tag	UNP A0A5M5BWR5
C	8	HIS	-	expression tag	UNP A0A5M5BWR5
C	9	HIS	-	expression tag	UNP A0A5M5BWR5
C	10	HIS	-	expression tag	UNP A0A5M5BWR5
C	11	SER	-	expression tag	UNP A0A5M5BWR5
C	12	SER	-	expression tag	UNP A0A5M5BWR5
C	13	GLY	-	expression tag	UNP A0A5M5BWR5
C	14	LEU	-	expression tag	UNP A0A5M5BWR5
C	15	VAL	-	expression tag	UNP A0A5M5BWR5
C	16	PRO	-	expression tag	UNP A0A5M5BWR5
C	17	ARG	-	expression tag	UNP A0A5M5BWR5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	18	GLY	-	expression tag	UNP A0A5M5BWR5
C	19	SER	-	expression tag	UNP A0A5M5BWR5
C	20	HIS	-	expression tag	UNP A0A5M5BWR5
C	21	MET	-	expression tag	UNP A0A5M5BWR5
C	22	ALA	-	expression tag	UNP A0A5M5BWR5
C	23	SER	-	expression tag	UNP A0A5M5BWR5
D	1	MET	-	initiating methionine	UNP A0A5M5BWR5
D	2	GLY	-	expression tag	UNP A0A5M5BWR5
D	3	SER	-	expression tag	UNP A0A5M5BWR5
D	4	SER	-	expression tag	UNP A0A5M5BWR5
D	5	HIS	-	expression tag	UNP A0A5M5BWR5
D	6	HIS	-	expression tag	UNP A0A5M5BWR5
D	7	HIS	-	expression tag	UNP A0A5M5BWR5
D	8	HIS	-	expression tag	UNP A0A5M5BWR5
D	9	HIS	-	expression tag	UNP A0A5M5BWR5
D	10	HIS	-	expression tag	UNP A0A5M5BWR5
D	11	SER	-	expression tag	UNP A0A5M5BWR5
D	12	SER	-	expression tag	UNP A0A5M5BWR5
D	13	GLY	-	expression tag	UNP A0A5M5BWR5
D	14	LEU	-	expression tag	UNP A0A5M5BWR5
D	15	VAL	-	expression tag	UNP A0A5M5BWR5
D	16	PRO	-	expression tag	UNP A0A5M5BWR5
D	17	ARG	-	expression tag	UNP A0A5M5BWR5
D	18	GLY	-	expression tag	UNP A0A5M5BWR5
D	19	SER	-	expression tag	UNP A0A5M5BWR5
D	20	HIS	-	expression tag	UNP A0A5M5BWR5
D	21	MET	-	expression tag	UNP A0A5M5BWR5
D	22	ALA	-	expression tag	UNP A0A5M5BWR5
D	23	SER	-	expression tag	UNP A0A5M5BWR5

- Molecule 2 is an oligosaccharide called 4-deoxy- $\alpha$ -L-erythro-hex-4-enopyranuronic acid-(1-4)- $\beta$ -D-mannopyranuronic acid-(1-4)- $\beta$ -D-mannopyranuronic acid.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	3	Total	C	O	0	0	0
			36	18	18			
2	F	3	Total	C	O	0	0	0
			36	18	18			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	G	3	Total	C	O	0	0	0
			36	18	18			
2	H	3	Total	C	O	0	0	0
			36	18	18			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

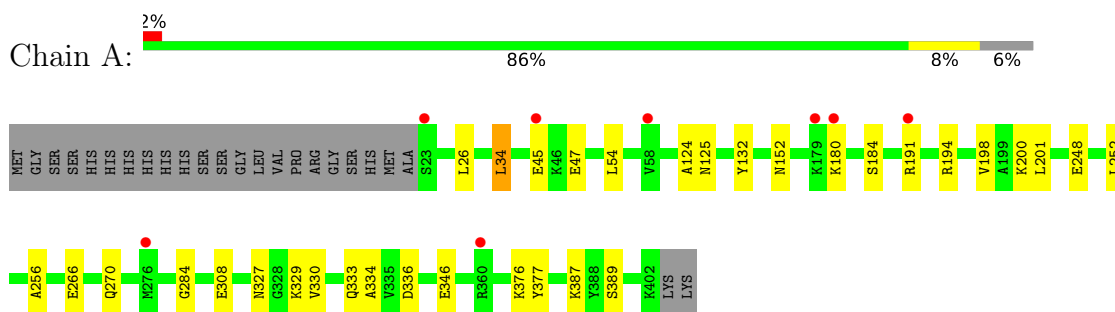
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	220	Total	O	0	0
			220	220		
4	B	213	Total	O	0	0
			213	213		
4	C	150	Total	O	0	0
			150	150		
4	D	153	Total	O	0	0
			153	153		

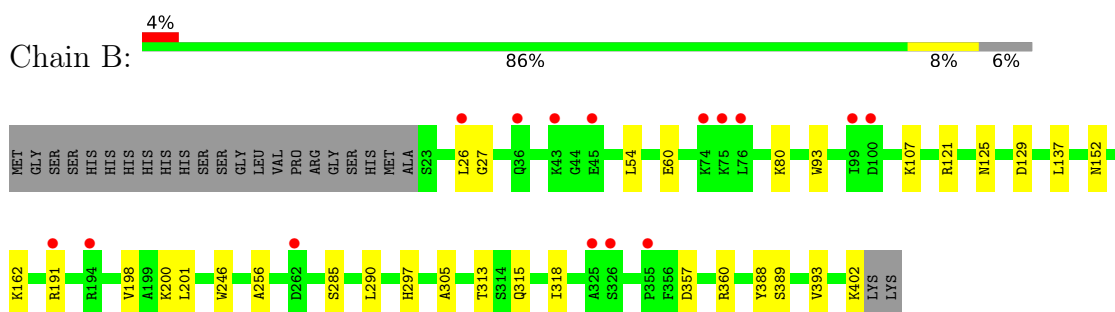
### 3 Residue-property plots [i](#)

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.

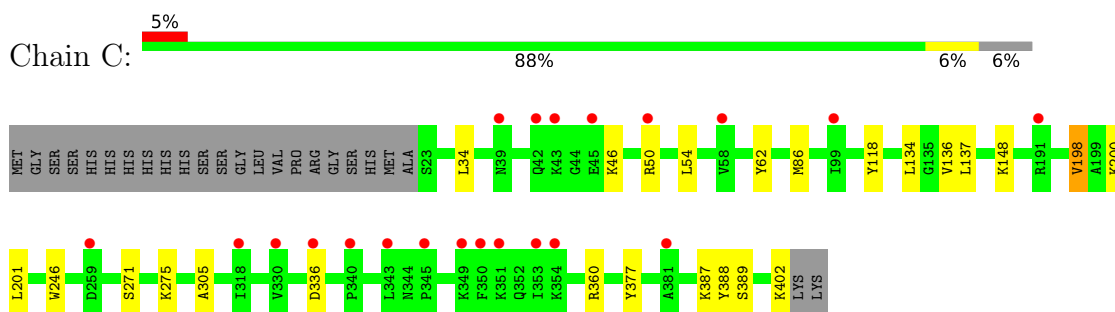
- Molecule 1: Alginate lyase family protein



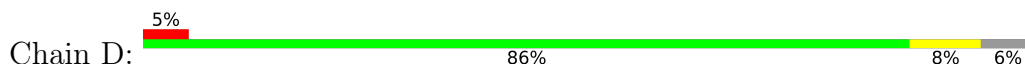
- Molecule 1: Alginate lyase family protein



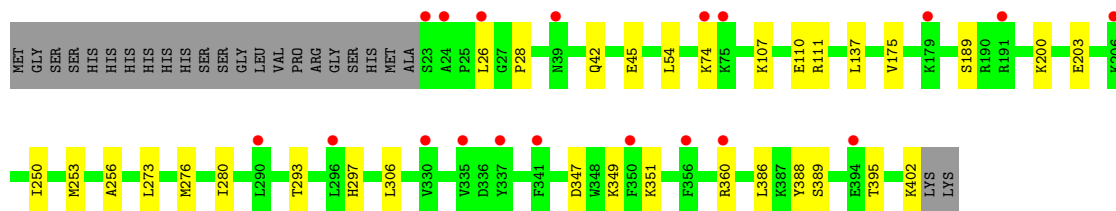
- Molecule 1: Alginate lyase family protein



- Molecule 1: Alginate lyase family protein







- Molecule 2: 4-deoxy-alpha-L-erythro-hex-4-enopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid

Chain E:  100%

BEH1  
BEH2  
MAW3

- Molecule 2: 4-deoxy-alpha-L-erythro-hex-4-enopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid

Chain F:  100%


BEH1  
BEH2  
MAW3

- Molecule 2: 4-deoxy-alpha-L-erythro-hex-4-enopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid

Chain G:  100%

BEH1  
BEH2  
MAW3

- Molecule 2: 4-deoxy-alpha-L-erythro-hex-4-enopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid

Chain H:  100%

BEH1  
BEH2  
MAW3

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	197.87Å 88.70Å 147.35Å 90.00° 120.39° 90.00°	Depositor
Resolution (Å)	58.48 – 1.76 58.48 – 1.76	Depositor EDS
% Data completeness (in resolution range)	81.4 (58.48-1.76) 81.4 (58.48-1.76)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.68 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, $R_{free}$	0.217 , 0.244 0.217 , 0.244	Depositor DCC
$R_{free}$ test set	10866 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 27.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13124	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.85% 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: BEM, MAW, SO4

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	0.37	0/3150	0.52	0/4268
1	B	0.37	0/3148	0.55	0/4266
1	C	0.37	0/3130	0.53	0/4242
1	D	0.36	0/3130	0.53	0/4242
All	All	0.37	0/12558	0.53	0/17018

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	3066	0	3041	22	0
1	B	3064	0	3044	25	0
1	C	3052	0	3022	18	0
1	D	3052	0	3022	19	0
2	E	36	0	19	0	0
2	F	36	0	19	0	0
2	G	36	0	19	0	0
2	H	36	0	19	0	0
3	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	5	0	0	0	0
4	A	220	0	0	7	0
4	B	213	0	0	8	0
4	C	150	0	0	2	0
4	D	153	0	0	2	0
All	All	13124	0	12205	85	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 (85) 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:387:LYS:NZ	4:A:501:HOH:O	1.87	1.07
1:D:42:GLN:NE2	4:D:601:HOH:O	2.05	0.89
1:B:360:ARG:NH1	4:B:603:HOH:O	2.13	0.74
1:C:360:ARG:NH1	4:C:501:HOH:O	2.21	0.72
1:B:162:LYS:NZ	4:B:602:HOH:O	2.12	0.71
1:B:198:VAL:HG13	1:B:201:LEU:HD12	1.71	0.71
1:D:200:LYS:HD2	4:D:665:HOH:O	1.91	0.69
1:A:198:VAL:HG13	1:A:201:LEU:HD12	1.75	0.69
1:B:256:ALA:O	4:B:601:HOH:O	2.11	0.68
1:C:86:MET:HE3	1:C:118:TYR:HE2	1.57	0.68
1:C:86:MET:HE3	1:C:118:TYR:CE2	2.30	0.66
1:D:386:LEU:HD13	1:D:395:THR:HB	1.80	0.62
1:D:276:MET:HE3	1:D:280:ILE:HD11	1.81	0.62
1:C:388:TYR:HA	1:C:402:LYS:HB3	1.81	0.61
1:C:336:ASP:OD1	1:C:377:TYR:OH	2.17	0.60
1:C:46:LYS:HE3	1:C:50:ARG:HH22	1.66	0.60
1:D:297:HIS:HA	1:D:360:ARG:HH22	1.67	0.60
1:C:198:VAL:HG22	1:C:201:LEU:HD12	1.84	0.59
1:D:200:LYS:HE2	1:D:203:GLU:OE2	2.04	0.58
1:C:387:LYS:HA	1:C:387:LYS:HE2	1.87	0.57
1:A:54:LEU:HD21	1:A:389:SER:HA	1.87	0.56
1:A:330:VAL:HG23	1:A:333:GLN:HG3	1.88	0.55
1:B:26:LEU:HB3	4:B:601:HOH:O	2.06	0.55
1:B:26:LEU:HA	1:B:315:GLN:NE2	2.22	0.55
1:D:189:SER:HB2	1:D:250:ILE:HD13	1.89	0.54
1:A:26:LEU:HG	1:A:256:ALA:HB1	1.90	0.53
1:A:200:LYS:NZ	4:A:505:HOH:O	2.28	0.51
1:A:152:ASN:ND2	4:A:507:HOH:O	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:SER:HB2	1:B:290:LEU:HD11	1.93	0.51
1:B:80:LYS:NZ	4:B:616:HOH:O	2.42	0.51
1:B:388:TYR:HA	1:B:402:LYS:HB3	1.92	0.51
1:C:50:ARG:N	1:C:50:ARG:HD2	2.26	0.51
1:A:124:ALA:HB3	1:A:191[B]:ARG:HH21	1.75	0.51
1:B:60:GLU:HG3	4:B:786:HOH:O	2.10	0.51
1:D:293:THR:HA	1:D:351:LYS:HD3	1.93	0.50
1:D:107:LYS:NZ	1:D:110:GLU:OE1	2.38	0.50
1:A:47:GLU:HG3	4:A:695:HOH:O	2.12	0.50
1:B:54:LEU:HD21	1:B:389:SER:HA	1.93	0.50
1:A:336:ASP:OD1	1:A:377:TYR:OH	2.28	0.49
1:A:346:GLU:OE2	1:A:346:GLU:N	2.35	0.48
1:C:46:LYS:HE3	1:C:50:ARG:NH2	2.28	0.48
1:C:34:LEU:HD11	1:C:136:VAL:HG13	1.95	0.48
1:C:271:SER:OG	1:C:275:LYS:NZ	2.45	0.48
1:D:276:MET:SD	1:D:306:LEU:HD13	2.53	0.47
1:B:129:ASP:HA	1:B:393:VAL:HG21	1.96	0.47
1:B:137:LEU:HA	1:B:137:LEU:HD23	1.74	0.47
1:A:125:ASN:CG	1:A:191[B]:ARG:HD2	2.38	0.47
1:B:93:TRP:CD1	1:B:107:LYS:HD3	2.51	0.46
1:B:357:ASP:HB3	1:B:360:ARG:HD3	1.97	0.46
1:C:46:LYS:O	1:C:50:ARG:HD3	2.16	0.46
1:D:26:LEU:HG	1:D:256:ALA:HB1	1.96	0.46
1:B:297:HIS:HA	1:B:360:ARG:HH22	1.81	0.45
1:A:327:ASN:ND2	1:A:329:LYS:HD2	2.32	0.45
1:A:180:LYS:NZ	4:A:511:HOH:O	2.46	0.45
1:A:194:ARG:HB2	4:A:502:HOH:O	2.17	0.44
1:A:266:GLU:O	1:A:270:GLN:HG3	2.17	0.44
1:B:27:GLY:H	1:B:315:GLN:HE22	1.65	0.44
1:D:54:LEU:HD21	1:D:389:SER:HA	1.99	0.44
1:B:121:ARG:HA	1:B:191[B]:ARG:NH2	2.32	0.44
1:D:347:ASP:O	1:D:349:LYS:HD2	2.17	0.44
1:A:34:LEU:HD12	1:A:34:LEU:HA	1.79	0.43
1:D:111:ARG:HH11	1:D:111:ARG:HG3	1.84	0.43
1:A:376:LYS:HE2	1:A:376:LYS:HB3	1.66	0.43
1:C:137:LEU:HD23	1:C:137:LEU:HA	1.76	0.43
1:B:200:LYS:HB2	1:B:200:LYS:HE2	1.72	0.43
1:D:388:TYR:HA	1:D:402:LYS:HB3	1.99	0.43
1:B:26:LEU:HG	1:B:256:ALA:HB1	2.01	0.43
1:B:162:LYS:HE2	4:B:745:HOH:O	2.18	0.43
1:A:284:GLY:O	1:A:334:ALA:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:LYS:HD3	1:D:74:LYS:HA	1.81	0.42
1:C:200:LYS:HG3	4:C:563:HOH:O	2.19	0.42
1:A:132:TYR:CD1	1:A:198:VAL:HG21	2.54	0.42
1:A:194:ARG:NH2	1:A:308:GLU:OE2	2.52	0.42
1:C:62:TYR:HB3	1:C:134:LEU:HD11	2.02	0.42
1:C:246:TRP:CD1	1:C:305:ALA:HB2	2.55	0.41
1:C:54:LEU:HD21	1:C:389:SER:HA	2.02	0.41
1:D:137:LEU:HD23	1:D:137:LEU:HA	1.75	0.41
1:D:28:PRO:HB3	1:D:253:MET:HG2	2.02	0.41
1:A:248:GLU:O	1:A:252:LEU:HG	2.20	0.41
1:B:125:ASN:ND2	1:B:191[A]:ARG:HD3	2.35	0.41
1:B:152:ASN:OD1	4:B:604:HOH:O	2.21	0.41
1:B:313:THR:HB	1:B:318:ILE:HB	2.03	0.41
1:B:246:TRP:CE2	1:B:305:ALA:HB2	2.56	0.40
1:D:273:LEU:HD23	1:D:273:LEU:HA	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	380/404 (94%)	374 (98%)	6 (2%)	0	100	100
1	B	380/404 (94%)	373 (98%)	7 (2%)	0	100	100
1	C	378/404 (94%)	371 (98%)	7 (2%)	0	100	100
1	D	378/404 (94%)	371 (98%)	7 (2%)	0	100	100
All	All	1516/1616 (94%)	1489 (98%)	27 (2%)	0	100	100

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	326/344 (95%)	323 (99%)	3 (1%)	75	65
1	B	326/344 (95%)	326 (100%)	0	100	100
1	C	324/344 (94%)	322 (99%)	2 (1%)	84	78
1	D	324/344 (94%)	322 (99%)	2 (1%)	84	78
All	All	1300/1376 (94%)	1293 (100%)	7 (0%)	86	82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	45	GLU
1	A	184	SER
1	C	148	LYS
1	C	198	VAL
1	D	45	GLU
1	D	175	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	173	GLN
1	A	279	GLN
1	A	375	GLN
1	B	36	GLN
1	B	42	GLN
1	B	125	ASN
1	B	173	GLN
1	B	315	GLN
1	B	358	GLN
1	C	173	GLN
1	C	232	GLN

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Mol	Chain	Res	Type
1	C	242	ASN
1	C	279	GLN
1	D	173	GLN
1	D	333	GLN
1	D	375	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	BEM	E	1	2	13,13,13	1.03	1 (7%)	18,19,19	1.49	2 (11%)
2	BEM	E	2	2	12,12,13	1.06	0	14,17,19	1.47	3 (21%)
2	MAW	E	3	2	10,11,12	1.33	1 (10%)	13,15,17	2.42	4 (30%)
2	BEM	F	1	2	13,13,13	0.98	0	18,19,19	1.18	1 (5%)
2	BEM	F	2	2	12,12,13	1.20	1 (8%)	14,17,19	1.33	3 (21%)
2	MAW	F	3	2	10,11,12	1.26	1 (10%)	13,15,17	2.01	2 (15%)
2	BEM	G	1	2	13,13,13	1.05	1 (7%)	18,19,19	1.31	2 (11%)
2	BEM	G	2	2	12,12,13	1.11	1 (8%)	14,17,19	1.08	0
2	MAW	G	3	2	10,11,12	1.23	0	13,15,17	1.86	3 (23%)
2	BEM	H	1	2	13,13,13	1.04	1 (7%)	18,19,19	1.39	2 (11%)
2	BEM	H	2	2	12,12,13	1.18	1 (8%)	14,17,19	0.88	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MAW	H	3	2	10,11,12	1.33	2 (20%)	13,15,17	2.04	2 (15%)

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	BEM	E	1	2	-	0/4/24/24	0/1/1/1
2	BEM	E	2	2	-	0/4/21/24	0/1/1/1
2	MAW	E	3	2	-	0/4/17/20	0/1/1/1
2	BEM	F	1	2	-	0/4/24/24	0/1/1/1
2	BEM	F	2	2	-	0/4/21/24	0/1/1/1
2	MAW	F	3	2	-	0/4/17/20	0/1/1/1
2	BEM	G	1	2	-	0/4/24/24	0/1/1/1
2	BEM	G	2	2	-	0/4/21/24	0/1/1/1
2	MAW	G	3	2	-	0/4/17/20	0/1/1/1
2	BEM	H	1	2	-	0/4/24/24	0/1/1/1
2	BEM	H	2	2	-	0/4/21/24	0/1/1/1
2	MAW	H	3	2	-	0/4/17/20	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3	MAW	C5-C6	2.74	1.55	1.48
2	F	2	BEM	O5-C1	-2.70	1.39	1.43
2	E	3	MAW	C5-C6	2.65	1.55	1.48
2	E	1	BEM	O6B-C6	-2.29	1.23	1.30
2	H	2	BEM	O6B-C6	-2.24	1.23	1.30
2	H	1	BEM	O6B-C6	-2.23	1.23	1.30
2	G	1	BEM	O6B-C6	-2.18	1.23	1.30
2	H	3	MAW	O5-C1	-2.13	1.42	1.45
2	H	3	MAW	C5-C6	2.09	1.53	1.48
2	G	2	BEM	O6B-C6	-2.05	1.23	1.30

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	MAW	O5-C5-C4	-6.35	119.45	124.81
2	F	3	MAW	O5-C5-C4	-5.34	120.30	124.81
2	G	3	MAW	O5-C5-C4	-4.55	120.97	124.81
2	H	3	MAW	O5-C5-C4	-4.47	121.04	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	3	MAW	C2-C3-C4	-3.87	107.02	112.32
2	E	3	MAW	C2-C3-C4	-3.75	107.19	112.32
2	E	1	BEM	O5-C5-C4	2.93	114.81	109.57
2	E	2	BEM	C3-C4-C5	-2.90	104.29	109.25
2	H	1	BEM	O5-C5-C4	2.63	114.27	109.57
2	G	1	BEM	O5-C5-C4	2.61	114.23	109.57
2	G	3	MAW	C2-C3-C4	-2.30	109.18	112.32
2	E	2	BEM	O6A-C6-C5	-2.28	112.46	120.81
2	E	1	BEM	O1-C1-C2	2.22	115.27	109.03
2	F	2	BEM	O6A-C6-C5	-2.20	112.74	120.81
2	F	2	BEM	O6B-C6-O6A	2.16	128.99	124.09
2	F	1	BEM	O5-C5-C4	2.15	113.41	109.57
2	E	2	BEM	O6B-C6-O6A	2.14	128.95	124.09
2	F	2	BEM	C1-C2-C3	2.14	112.30	109.67
2	G	1	BEM	O4-C4-C5	-2.13	104.97	109.74
2	G	3	MAW	O6B-C6-O6A	2.12	128.46	123.61
2	E	3	MAW	C3-C4-C5	-2.10	118.04	121.60
2	F	3	MAW	C2-C3-C4	-2.05	109.51	112.32
2	E	3	MAW	O6A-C6-C5	-2.03	115.10	120.48
2	H	1	BEM	O6A-C6-C5	-2.02	113.39	120.81

There are no chirality outliers.

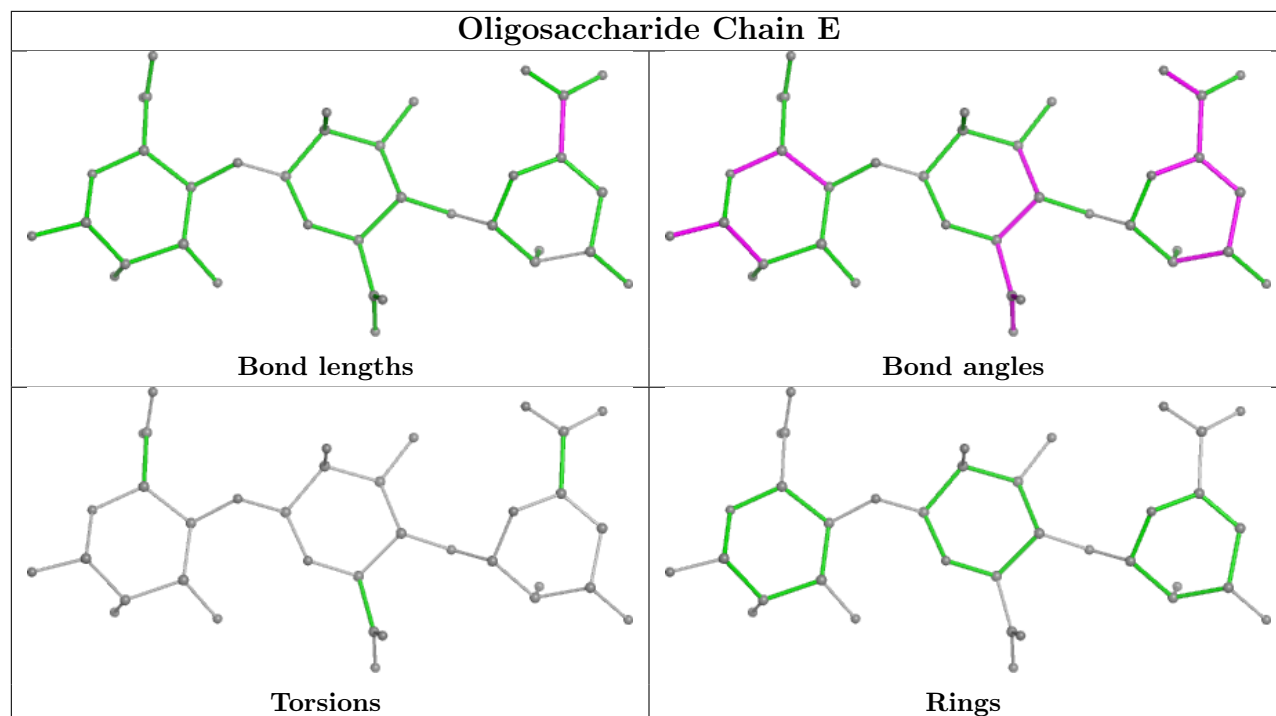
There are no torsion outliers.

There are no ring outliers.

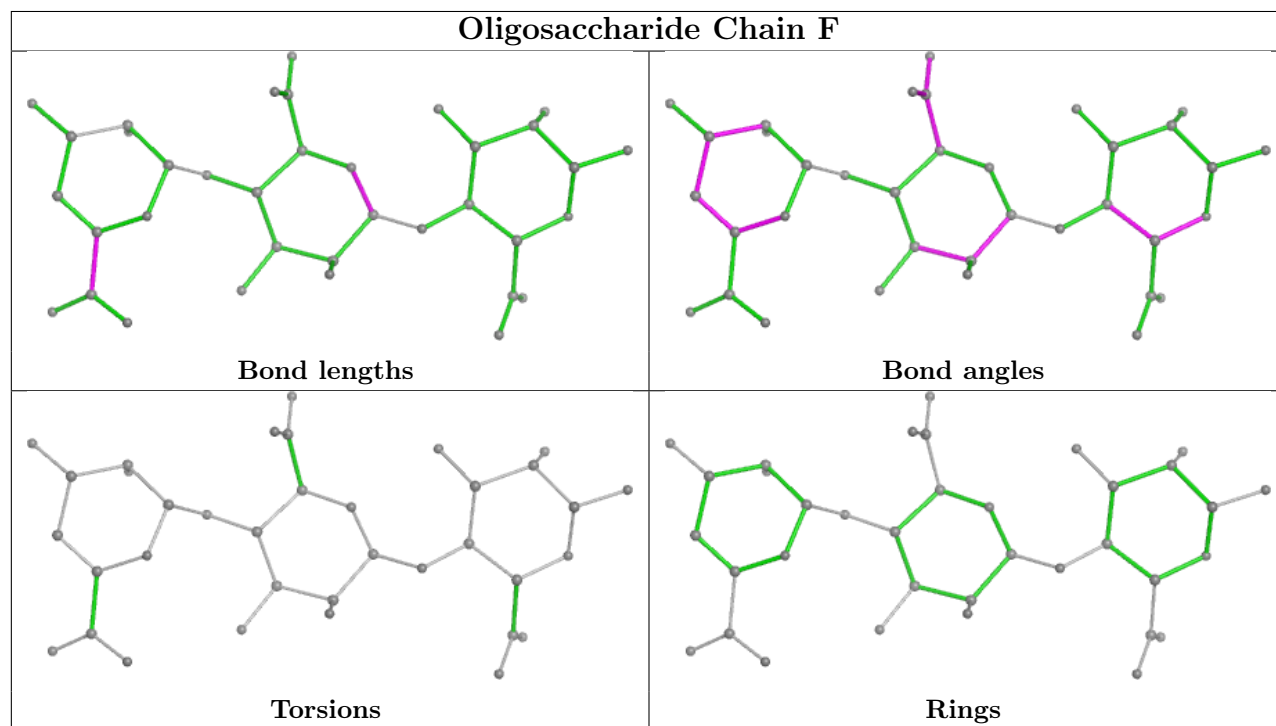
No monomer is involved in short contacts.

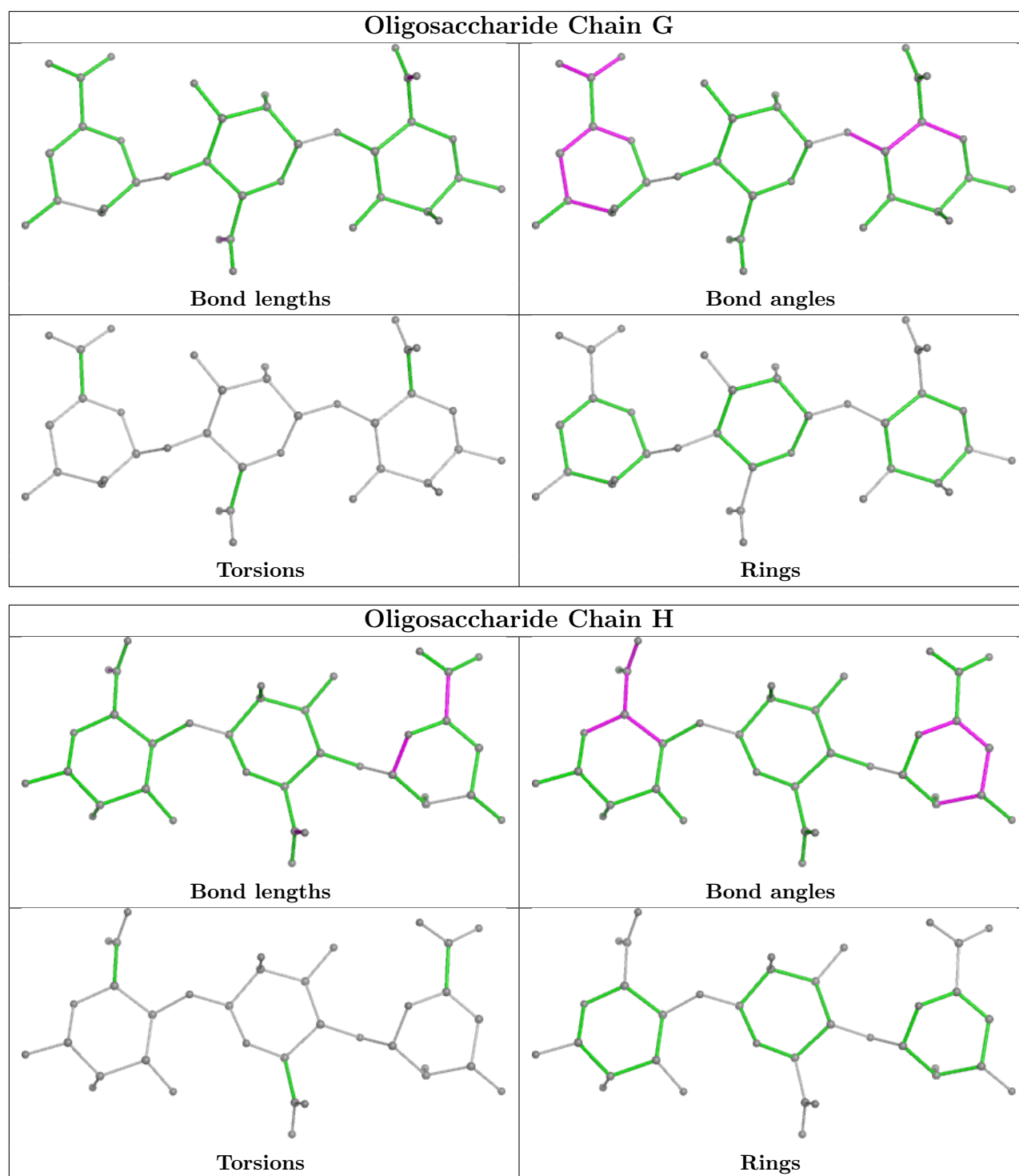
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

## Oligosaccharide Chain E



## Oligosaccharide Chain F





## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	D	501	-	4,4,4	0.66	0	6,6,6	0.07	0
3	SO4	B	501	-	4,4,4	0.66	0	6,6,6	0.18	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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	380/404 (94%)	0.35	8 (2%) 63 69	20, 32, 43, 53	2 (0%)
1	B	380/404 (94%)	0.40	15 (3%) 44 50	17, 33, 44, 54	2 (0%)
1	C	380/404 (94%)	0.56	21 (5%) 32 35	25, 36, 48, 58	0
1	D	380/404 (94%)	0.58	19 (5%) 35 38	24, 37, 49, 55	0
All	All	1520/1616 (94%)	0.47	63 (4%) 42 48	17, 34, 47, 58	4 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	LYS	3.8
1	C	50	ARG	3.6
1	B	191[A]	ARG	3.3
1	D	23	SER	3.2
1	D	360	ARG	3.1
1	D	39	ASN	3.0
1	C	259	ASP	3.0
1	D	394	GLU	3.0
1	C	99	ILE	3.0
1	B	26	LEU	2.9
1	D	26	LEU	2.9
1	C	42	GLN	2.7
1	D	74	LYS	2.7
1	B	36	GLN	2.7
1	B	326	SER	2.7
1	B	75	LYS	2.7
1	C	350	PHE	2.6
1	B	355	PRO	2.6
1	C	343	LEU	2.6
1	C	43	LYS	2.6
1	B	194	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	337	TYR	2.5
1	A	360	ARG	2.5
1	B	325	ALA	2.5
1	A	276	MET	2.5
1	D	341	PHE	2.4
1	D	356	PHE	2.3
1	D	335	VAL	2.3
1	B	100	ASP	2.3
1	A	179	LYS	2.3
1	C	345	PRO	2.2
1	A	45	GLU	2.2
1	C	58	VAL	2.2
1	B	262	ASP	2.2
1	C	39	ASN	2.2
1	C	191	ARG	2.2
1	C	45	GLU	2.2
1	A	58	VAL	2.2
1	D	290	LEU	2.2
1	D	24	ALA	2.2
1	B	43	LYS	2.2
1	D	75	LYS	2.2
1	A	23	SER	2.1
1	A	180	LYS	2.1
1	C	381	ALA	2.1
1	B	99	ILE	2.1
1	C	340	PRO	2.1
1	D	191	ARG	2.1
1	C	354	LYS	2.1
1	D	206	LYS	2.1
1	B	45	GLU	2.1
1	C	351	LYS	2.1
1	B	76	LEU	2.1
1	C	330	VAL	2.1
1	C	336	ASP	2.1
1	C	353	ILE	2.1
1	D	350	PHE	2.1
1	C	349	LYS	2.1
1	D	296	LEU	2.1
1	D	330	VAL	2.1
1	A	191[A]	ARG	2.0
1	D	179	LYS	2.0
1	C	318	ILE	2.0

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

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

## 6.3 Carbohydrates ⓘ

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.

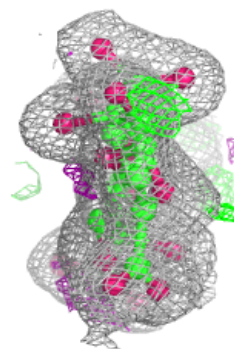
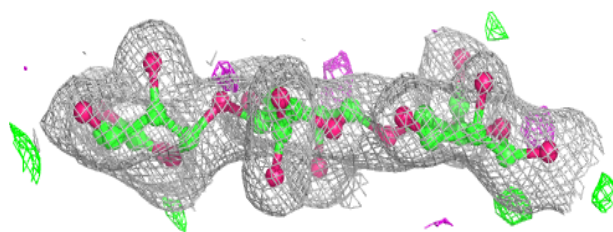
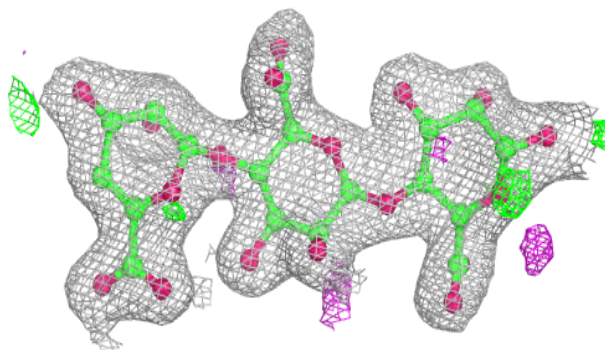
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BEM	H	1	13/13	0.84	0.13	40,46,54,54	0
2	BEM	E	1	13/13	0.90	0.09	32,39,46,51	0
2	BEM	F	1	13/13	0.92	0.09	35,41,51,51	0
2	BEM	G	1	13/13	0.93	0.09	38,46,53,56	0
2	BEM	H	2	12/13	0.93	0.09	32,37,39,39	0
2	MAW	H	3	11/12	0.95	0.08	30,34,36,36	0
2	BEM	G	2	12/13	0.96	0.06	32,37,39,40	0
2	MAW	G	3	11/12	0.96	0.07	31,34,36,36	0
2	BEM	E	2	12/13	0.96	0.07	26,30,33,35	0
2	MAW	F	3	11/12	0.96	0.06	26,29,31,31	0
2	MAW	E	3	11/12	0.96	0.06	26,27,30,30	0
2	BEM	F	2	12/13	0.97	0.05	30,32,34,35	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.

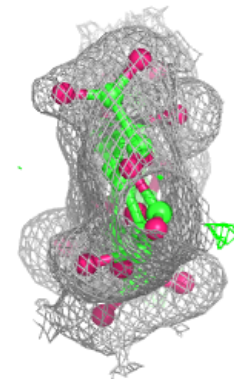
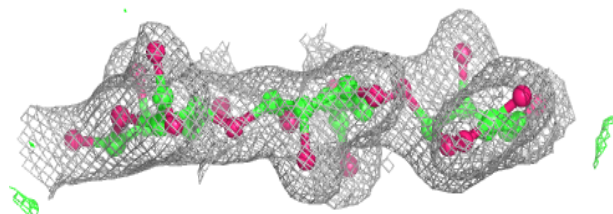
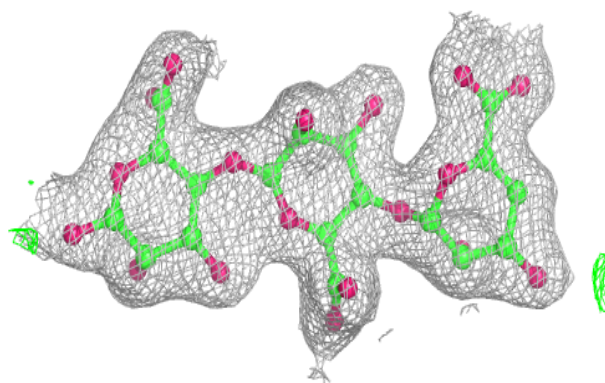


**Electron density around Chain E:**

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

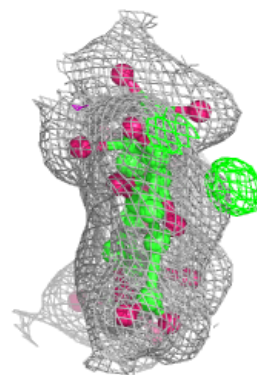
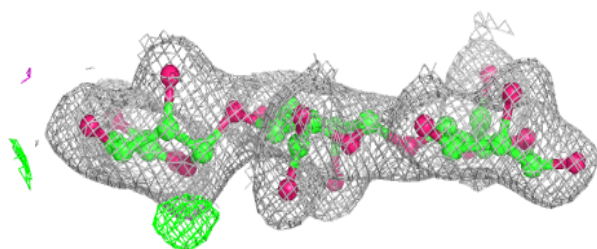
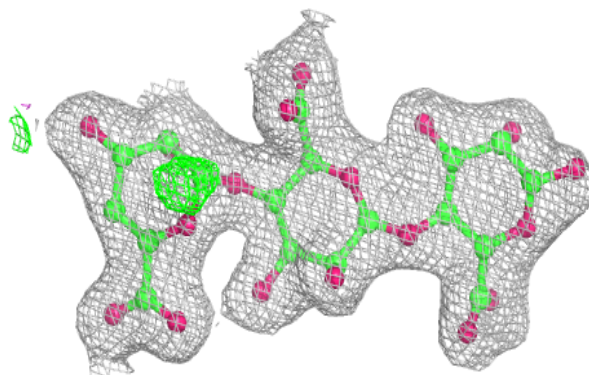
**Electron density around Chain F:**

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

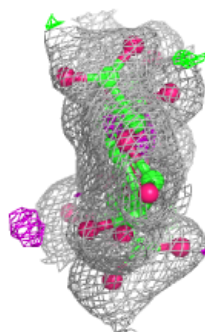
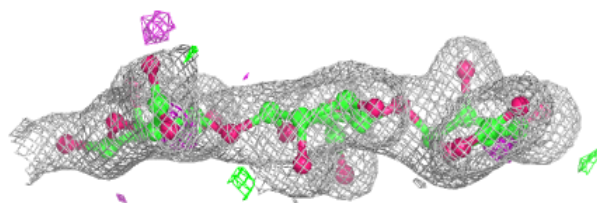
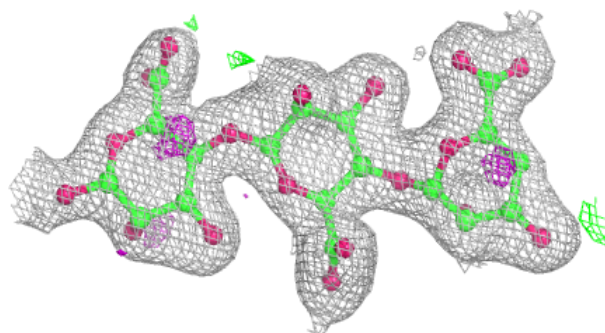


**Electron density around Chain G:**

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

**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)



## 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
3	SO4	D	501	5/5	0.34	0.17	103,106,122,123	0
3	SO4	B	501	5/5	0.83	0.17	36,41,45,46	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.