



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 04:23 AM BST

PDB ID : 5HYI  
Title : Glycosylated, disulfide-linked Hole-Hole Fc fragment  
Authors : Kuglstatter, A.; Stihle, M.; Benz, J.  
Deposited on : 2016-02-01  
Resolution : 2.90 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

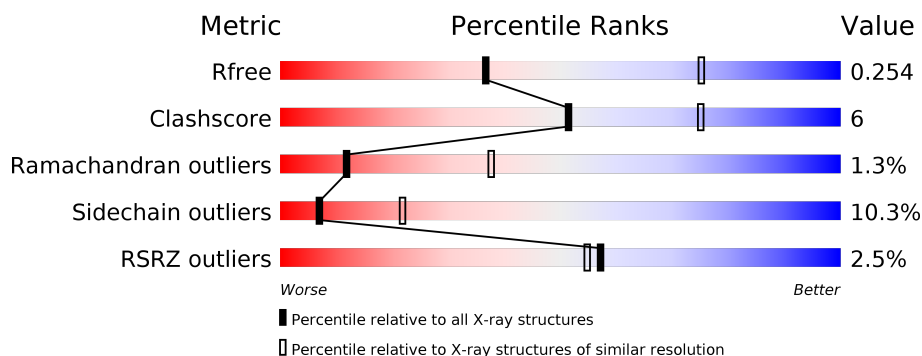
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	227	<div> <div style="width: 74%;"></div> <div style="width: 18%;"></div> <div style="width: 8%;"></div> </div>
1	B	227	<div> <div style="width: 3%;"></div> <div style="width: 66%;"></div> <div style="width: 23%;"></div> <div style="width: 8%;"></div> </div>
1	C	227	<div> <div style="width: 6%;"></div> <div style="width: 67%;"></div> <div style="width: 23%;"></div> <div style="width: 8%;"></div> </div>
1	D	227	<div> <div style="width: 70%;"></div> <div style="width: 20%;"></div> <div style="width: 8%;"></div> </div>
2	E	9	<div> <div style="width: 22%;"></div> <div style="width: 67%;"></div> <div style="width: 11%;"></div> </div>
2	F	9	<div> <div style="width: 11%;"></div> <div style="width: 89%;"></div> </div>

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Mol	Chain	Length	Quality of chain
2	G	9	 44% 44% 11%
2	H	9	 44% 33% 22%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7251 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 Ig gamma-1 chain C region.

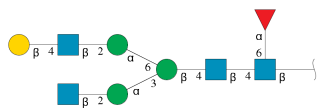
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1656	1050	281	318	7			
1	B	209	Total	C	N	O	S	0	0	0
			1653	1047	281	318	7			
1	C	208	Total	C	N	O	S	0	0	0
			1649	1045	280	317	7			
1	D	209	Total	C	N	O	S	0	0	0
			1653	1047	281	318	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	349	CYS	TYR	engineered mutation	UNP P01857
A	366	SER	THR	engineered mutation	UNP P01857
A	368	ALA	LEU	engineered mutation	UNP P01857
A	407	VAL	TYR	engineered mutation	UNP P01857
B	349	CYS	TYR	engineered mutation	UNP P01857
B	366	SER	THR	engineered mutation	UNP P01857
B	368	ALA	LEU	engineered mutation	UNP P01857
B	407	VAL	TYR	engineered mutation	UNP P01857
C	349	CYS	TYR	engineered mutation	UNP P01857
C	366	SER	THR	engineered mutation	UNP P01857
C	368	ALA	LEU	engineered mutation	UNP P01857
C	407	VAL	TYR	engineered mutation	UNP P01857
D	349	CYS	TYR	engineered mutation	UNP P01857
D	366	SER	THR	engineered mutation	UNP P01857
D	368	ALA	LEU	engineered mutation	UNP P01857
D	407	VAL	TYR	engineered mutation	UNP P01857

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

-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	9	Total	C	N	O	0	0	0
			110	62	4	44			
2	F	9	Total	C	N	O	0	0	0
			110	62	4	44			
2	G	9	Total	C	N	O	0	0	0
			110	62	4	44			
2	H	9	Total	C	N	O	0	0	0
			110	62	4	44			

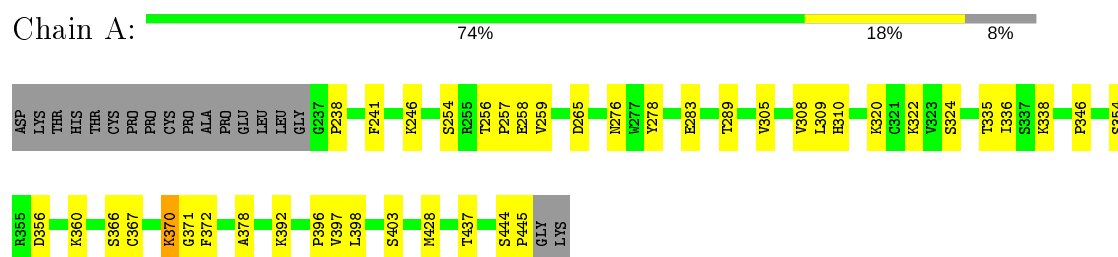
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total	O	0	0
			66	66		
3	B	29	Total	O	0	0
			29	29		
3	C	33	Total	O	0	0
			33	33		
3	D	72	Total	O	0	0
			72	72		

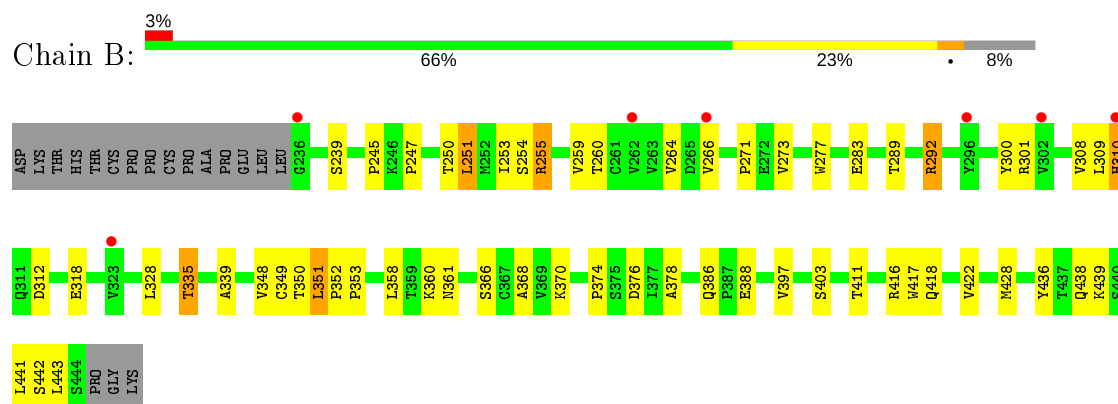
### 3 Residue-property plots

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.

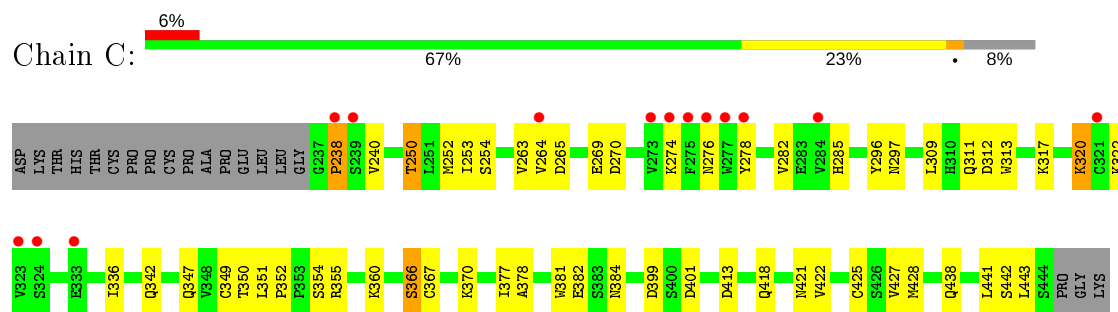
- Molecule 1: Ig gamma-1 chain C region



- Molecule 1: Ig gamma-1 chain C region

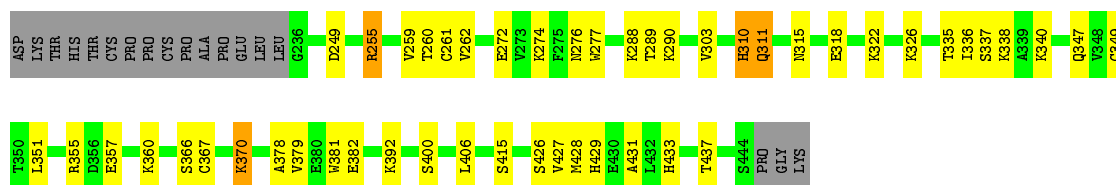


- Molecule 1: Ig gamma-1 chain C region



- Molecule 1: Ig gamma-1 chain C region





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

Chain E: 22% 67% 11%



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

Chain F: 11% 89%



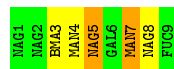
- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 44% 44% 11%



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

Chain H: 44% 33% 22%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.28Å 105.66Å 134.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 2.90 49.17 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.15-2.90) 99.5 (49.17-2.90)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, $R_{free}$	0.175 , 0.235 0.197 , 0.254	Depositor DCC
$R_{free}$ test set	1677 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.9	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 67.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7251	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.01% 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: MAN, GAL, BMA, NAG, FUC

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	0.58	0/1701	0.79	0/2318
1	B	0.52	0/1697	0.75	0/2311
1	C	0.53	0/1693	0.72	0/2306
1	D	0.56	0/1697	0.78	0/2311
All	All	0.55	0/6788	0.76	0/9246

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	1656	0	1624	14	0
1	B	1653	0	1620	25	0
1	C	1649	0	1617	24	0
1	D	1653	0	1620	21	0
2	E	110	0	94	1	0
2	F	110	0	94	0	0
2	G	110	0	94	1	0
2	H	110	0	94	2	0
3	A	66	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	29	0	0	1	0
3	C	33	0	0	1	0
3	D	72	0	0	1	0
All	All	7251	0	6857	78	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 6.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:VAL:HG22	1:B:442:SER:HB3	1.63	0.79
1:B:386:GLN:HG2	1:D:355:ARG:HG2	1.70	0.74
1:D:259:VAL:HG13	1:D:336:ILE:HD11	1.75	0.69
1:C:278:TYR:HB2	1:C:320:LYS:HB2	1.76	0.67
1:A:278:TYR:HB2	1:A:320:LYS:HB3	1.79	0.64
1:C:347:GLN:HB3	1:D:351:LEU:HD22	1.79	0.64
1:A:259:VAL:HG13	1:A:336:ILE:HD11	1.79	0.64
1:C:367:CYS:HB2	1:C:381:TRP:CZ2	2.33	0.63
1:D:379:VAL:HG22	1:D:427:VAL:HG22	1.83	0.60
1:D:378:ALA:HB3	1:D:428:MET:HB2	1.86	0.57
1:C:238:PRO:HA	1:C:265:ASP:HB2	1.87	0.57
1:B:348:VAL:HB	1:B:439:LYS:HG3	1.85	0.56
1:B:308:VAL:HA	3:B:615:HOH:O	2.05	0.56
1:D:249:ASP:HA	1:D:255:ARG:HG3	1.87	0.56
1:A:378:ALA:HB3	1:A:428:MET:HB2	1.88	0.55
1:C:425:CYS:O	1:C:438:GLN:HA	2.06	0.55
1:D:274:LYS:NZ	1:D:276:ASN:HD21	2.05	0.55
1:D:429:HIS:HD2	1:D:431:ALA:H	1.55	0.55
1:C:378:ALA:HB3	1:C:428:MET:HB2	1.89	0.55
1:C:350:THR:HB	1:C:441:LEU:HD22	1.88	0.54
1:A:276:ASN:HB2	1:A:322:LYS:HB3	1.88	0.54
1:C:418:GLN:HA	1:C:443:LEU:HD22	1.89	0.54
1:D:276:ASN:HB2	1:D:322:LYS:HB3	1.89	0.53
1:C:355:ARG:HH22	1:D:433:HIS:HB2	1.73	0.53
1:C:250:THR:HG21	1:C:313:TRP:CD1	2.44	0.53
1:B:247:PRO:O	1:B:251:LEU:HD22	2.08	0.52
1:C:276:ASN:HB2	1:C:322:LYS:HB3	1.91	0.52
1:D:351:LEU:HB2	1:D:366:SER:HB2	1.89	0.52
1:D:262:VAL:HG22	1:D:303:VAL:HG22	1.91	0.51
1:B:352:PRO:HB2	1:B:353:PRO:CD	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:PRO:HA	1:A:265:ASP:HB2	1.95	0.49
1:B:339:ALA:HB3	1:B:374:PRO:HB3	1.94	0.49
1:C:366:SER:HB3	1:D:370:LYS:HD3	1.95	0.49
1:A:278:TYR:CE2	1:A:283:GLU:HB2	2.48	0.48
1:B:378:ALA:HB3	1:B:428:MET:HB2	1.95	0.48
1:B:350:THR:HB	1:B:441:LEU:HD22	1.96	0.47
1:A:370:LYS:HG2	1:B:351:LEU:HD13	1.96	0.47
1:D:429:HIS:CD2	1:D:431:ALA:H	2.31	0.47
1:C:377:ILE:HD11	1:C:427:VAL:HG13	1.96	0.47
1:D:318:GLU:HG2	1:D:335:THR:CG2	2.45	0.47
1:B:247:PRO:HA	1:B:250:THR:HG22	1.97	0.47
1:C:312:ASP:HB3	1:C:317:LYS:HD2	1.96	0.47
1:D:311:GLN:HB3	3:D:605:HOH:O	2.14	0.47
1:C:351:LEU:HD22	1:D:347:GLN:HB3	1.96	0.47
1:B:277:TRP:O	1:B:283:GLU:HA	2.14	0.47
1:B:247:PRO:O	1:B:250:THR:HG22	2.16	0.46
1:B:264:VAL:HG12	1:B:301:ARG:HG3	1.98	0.46
1:D:367:CYS:HB2	1:D:381:TRP:CZ2	2.50	0.46
1:C:422:VAL:HG22	1:C:442:SER:HB3	1.99	0.45
1:C:278:TYR:HB2	1:C:320:LYS:HD2	1.99	0.45
1:A:241:PHE:CZ	2:E:2:NAG:H61	2.52	0.45
1:A:371:GLY:HA2	1:A:403:SER:OG	2.17	0.45
1:B:255:ARG:N	1:B:255:ARG:HD2	2.32	0.44
1:A:346:PRO:HB3	1:A:372:PHE:HB3	2.00	0.44
1:C:240:VAL:HG22	1:C:263:VAL:HG12	2.00	0.43
1:C:351:LEU:HA	1:C:352:PRO:HD3	1.92	0.43
1:C:250:THR:HG21	1:C:313:TRP:HD1	1.82	0.43
2:H:3:BMA:H2	2:H:7:MAN:O5	2.19	0.43
1:C:384:ASN:HB3	3:C:607:HOH:O	2.19	0.43
1:B:318:GLU:HG2	1:B:335:THR:HG22	2.00	0.42
1:A:258:GLU:HB2	1:A:305:VAL:HG12	2.02	0.42
1:B:266:VAL:HB	1:B:300:TYR:HB2	2.01	0.42
1:D:260:THR:HG21	2:H:5:NAG:H61	2.01	0.42
1:B:271:PRO:O	1:B:273:VAL:HG23	2.19	0.42
1:A:444:SER:O	1:A:445:PRO:C	2.58	0.42
1:B:417:TRP:NE1	1:B:443:LEU:HD13	2.35	0.42
1:C:296:TYR:CD2	2:G:9:FUC:H62	2.55	0.42
1:B:245:PRO:HD3	1:B:259:VAL:HG22	2.01	0.41
1:C:399:ASP:HB3	1:C:401:ASP:OD1	2.20	0.41
1:B:349:CYS:HB3	1:B:368:ALA:HB3	2.02	0.41
1:B:388:GLU:CD	1:B:416:ARG:HH22	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:TYR:CE1	1:B:438:GLN:HG3	2.55	0.41
1:D:261:CYS:HB2	1:D:277:TRP:CZ2	2.55	0.41
1:A:257:PRO:HB2	1:A:308:VAL:HG22	2.03	0.41
1:B:292:ARG:HB2	1:B:300:TYR:HD1	1.86	0.41
1:C:351:LEU:HB2	1:C:366:SER:HB2	2.03	0.41
1:D:406:LEU:HD12	1:D:406:LEU:C	2.42	0.40
1:A:397:VAL:HG11	1:B:397:VAL:HG21	2.03	0.40

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	207/227 (91%)	197 (95%)	9 (4%)	1 (0%)	29	61
1	B	207/227 (91%)	190 (92%)	11 (5%)	6 (3%)	4	18
1	C	206/227 (91%)	186 (90%)	18 (9%)	2 (1%)	15	45
1	D	207/227 (91%)	197 (95%)	8 (4%)	2 (1%)	15	45
All	All	827/908 (91%)	770 (93%)	46 (6%)	11 (1%)	12	37

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	HIS
1	B	376	ASP
1	B	254	SER
1	B	310	HIS
1	D	310	HIS
1	D	311	GLN
1	B	292	ARG
1	B	253	ILE

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Mol	Chain	Res	Type
1	B	358	LEU
1	C	297	ASN
1	C	238	PRO

### 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	194/209 (93%)	176 (91%)	18 (9%)	9	27
1	B	193/209 (92%)	175 (91%)	18 (9%)	9	27
1	C	193/209 (92%)	170 (88%)	23 (12%)	5	15
1	D	193/209 (92%)	172 (89%)	21 (11%)	6	19
All	All	773/836 (92%)	693 (90%)	80 (10%)	7	22

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	LYS
1	A	254	SER
1	A	256	THR
1	A	289	THR
1	A	309	LEU
1	A	324	SER
1	A	335	THR
1	A	338	LYS
1	A	354	SER
1	A	356	ASP
1	A	360	LYS
1	A	366	SER
1	A	367	CYS
1	A	370	LYS
1	A	392	LYS
1	A	396	PRO
1	A	398	LEU
1	A	437	THR

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Mol	Chain	Res	Type
1	B	239	SER
1	B	251	LEU
1	B	255	ARG
1	B	260	THR
1	B	289	THR
1	B	309	LEU
1	B	310	HIS
1	B	312	ASP
1	B	328	LEU
1	B	335	THR
1	B	351	LEU
1	B	360	LYS
1	B	361	ASN
1	B	366	SER
1	B	370	LYS
1	B	403	SER
1	B	411	THR
1	B	418	GLN
1	C	250	THR
1	C	252	MET
1	C	253	ILE
1	C	254	SER
1	C	264	VAL
1	C	269	GLU
1	C	270	ASP
1	C	274	LYS
1	C	282	VAL
1	C	285	HIS
1	C	309	LEU
1	C	311	GLN
1	C	320	LYS
1	C	336	ILE
1	C	342	GLN
1	C	349	CYS
1	C	354	SER
1	C	360	LYS
1	C	366	SER
1	C	370	LYS
1	C	382	GLU
1	C	413	ASP
1	C	421	ASN
1	D	255	ARG

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Mol	Chain	Res	Type
1	D	272	GLU
1	D	288	LYS
1	D	289	THR
1	D	290	LYS
1	D	310	HIS
1	D	315	ASN
1	D	326	LYS
1	D	337	SER
1	D	338	LYS
1	D	340	LYS
1	D	349	CYS
1	D	357	GLU
1	D	360	LYS
1	D	370	LYS
1	D	382	GLU
1	D	392	LYS
1	D	400	SER
1	D	415	SER
1	D	426	SER
1	D	437	THR

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

Mol	Chain	Res	Type
1	B	361	ASN
1	C	276	ASN
1	C	347	GLN
1	C	421	ASN
1	D	276	ASN
1	D	311	GLN
1	D	429	HIS
1	D	434	ASN
1	D	435	HIS

### 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 ⓘ

36 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	E	1	1,2	14,14,15	0.27	0	17,19,21	0.71	1 (5%)
2	NAG	E	2	2	14,14,15	0.33	0	17,19,21	0.82	1 (5%)
2	BMA	E	3	2	11,11,12	0.43	0	15,15,17	0.74	0
2	MAN	E	4	2	11,11,12	0.36	0	15,15,17	0.88	2 (13%)
2	NAG	E	5	2	14,14,15	0.25	0	17,19,21	0.90	1 (5%)
2	GAL	E	6	2	11,11,12	0.46	0	15,15,17	0.69	0
2	MAN	E	7	2	11,11,12	0.75	1 (9%)	15,15,17	1.78	2 (13%)
2	NAG	E	8	2	14,14,15	0.39	0	17,19,21	1.64	2 (11%)
2	FUC	E	9	2	10,10,11	0.50	0	14,14,16	0.86	1 (7%)
2	NAG	F	1	1,2	14,14,15	0.30	0	17,19,21	0.80	1 (5%)
2	NAG	F	2	2	14,14,15	0.34	0	17,19,21	0.67	1 (5%)
2	BMA	F	3	2	11,11,12	0.28	0	15,15,17	0.86	1 (6%)
2	MAN	F	4	2	11,11,12	0.59	0	15,15,17	1.05	2 (13%)
2	NAG	F	5	2	14,14,15	0.34	0	17,19,21	1.04	2 (11%)
2	GAL	F	6	2	11,11,12	0.44	0	15,15,17	0.65	0
2	MAN	F	7	2	11,11,12	0.51	0	15,15,17	1.35	3 (20%)
2	NAG	F	8	2	14,14,15	0.26	0	17,19,21	1.14	2 (11%)
2	FUC	F	9	2	10,10,11	0.52	0	14,14,16	0.87	1 (7%)
2	NAG	G	1	1,2	14,14,15	0.29	0	17,19,21	0.96	1 (5%)
2	NAG	G	2	2	14,14,15	0.38	0	17,19,21	0.65	0
2	BMA	G	3	2	11,11,12	0.51	0	15,15,17	0.71	0
2	MAN	G	4	2	11,11,12	0.40	0	15,15,17	1.10	1 (6%)
2	NAG	G	5	2	14,14,15	0.28	0	17,19,21	1.56	3 (17%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GAL	G	6	2	11,11,12	0.40	0	15,15,17	0.60	0
2	MAN	G	7	2	11,11,12	0.44	0	15,15,17	0.79	1 (6%)
2	NAG	G	8	2	14,14,15	0.36	0	17,19,21	0.59	0
2	FUC	G	9	2	10,10,11	0.43	0	14,14,16	1.38	2 (14%)
2	NAG	H	1	1,2	14,14,15	0.29	0	17,19,21	0.59	0
2	NAG	H	2	2	14,14,15	0.29	0	17,19,21	0.57	0
2	BMA	H	3	2	11,11,12	0.37	0	15,15,17	0.77	0
2	MAN	H	4	2	11,11,12	0.35	0	15,15,17	0.88	1 (6%)
2	NAG	H	5	2	14,14,15	0.37	0	17,19,21	0.89	1 (5%)
2	GAL	H	6	2	11,11,12	0.50	0	15,15,17	0.70	0
2	MAN	H	7	2	11,11,12	0.62	0	15,15,17	1.64	2 (13%)
2	NAG	H	8	2	14,14,15	0.31	0	17,19,21	0.75	1 (5%)
2	FUC	H	9	2	10,10,11	0.40	0	14,14,16	0.74	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	0/1/1/1
2	NAG	E	5	2	-	0/6/23/26	0/1/1/1
2	GAL	E	6	2	-	0/2/19/22	0/1/1/1
2	MAN	E	7	2	-	1/2/19/22	0/1/1/1
2	NAG	E	8	2	-	2/6/23/26	0/1/1/1
2	FUC	E	9	2	-	-	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	MAN	F	4	2	-	1/2/19/22	0/1/1/1
2	NAG	F	5	2	-	0/6/23/26	0/1/1/1
2	GAL	F	6	2	-	0/2/19/22	0/1/1/1
2	MAN	F	7	2	-	0/2/19/22	0/1/1/1
2	NAG	F	8	2	-	0/6/23/26	0/1/1/1
2	FUC	F	9	2	-	-	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
2	MAN	G	4	2	-	0/2/19/22	0/1/1/1
2	NAG	G	5	2	-	5/6/23/26	0/1/1/1
2	GAL	G	6	2	-	0/2/19/22	0/1/1/1
2	MAN	G	7	2	-	2/2/19/22	0/1/1/1
2	NAG	G	8	2	-	1/6/23/26	0/1/1/1
2	FUC	G	9	2	-	-	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	BMA	H	3	2	-	1/2/19/22	0/1/1/1
2	MAN	H	4	2	-	0/2/19/22	0/1/1/1
2	NAG	H	5	2	-	0/6/23/26	0/1/1/1
2	GAL	H	6	2	-	0/2/19/22	0/1/1/1
2	MAN	H	7	2	-	1/2/19/22	0/1/1/1
2	NAG	H	8	2	-	0/6/23/26	0/1/1/1
2	FUC	H	9	2	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	7	MAN	C1-C2	2.08	1.56	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	8	NAG	C1-O5-C5	5.48	119.62	112.19
2	E	7	MAN	C1-O5-C5	4.67	118.52	112.19
2	G	5	NAG	O5-C1-C2	-4.00	104.98	111.29
2	H	7	MAN	C1-O5-C5	3.83	117.38	112.19
2	G	9	FUC	C3-C4-C5	3.69	115.52	109.77
2	H	7	MAN	C1-C2-C3	3.66	114.16	109.67
2	G	5	NAG	C1-C2-N2	3.62	116.68	110.49
2	E	7	MAN	C1-C2-C3	3.50	113.97	109.67
2	F	8	NAG	O5-C1-C2	-3.19	106.25	111.29
2	H	4	MAN	C1-O5-C5	3.13	116.44	112.19
2	F	7	MAN	O2-C2-C3	3.10	116.35	110.14
2	F	4	MAN	C1-C2-C3	2.93	113.27	109.67
2	F	3	BMA	C1-O5-C5	2.83	116.02	112.19
2	G	4	MAN	C1-O5-C5	2.80	115.99	112.19
2	E	2	NAG	O5-C1-C2	-2.68	107.06	111.29
2	F	8	NAG	C1-O5-C5	2.60	115.71	112.19
2	G	9	FUC	C1-O5-C5	2.56	118.58	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C1-O5-C5	2.55	115.65	112.19
2	F	7	MAN	C1-C2-C3	2.49	112.72	109.67
2	H	5	NAG	O5-C1-C2	-2.46	107.41	111.29
2	E	4	MAN	C1-O5-C5	2.43	115.48	112.19
2	F	9	FUC	C1-O5-C5	2.32	118.04	112.78
2	G	1	NAG	C1-C2-N2	2.25	114.33	110.49
2	H	8	NAG	C1-C2-N2	-2.24	106.67	110.49
2	E	5	NAG	O5-C1-C2	-2.23	107.76	111.29
2	F	5	NAG	C1-O5-C5	2.23	115.22	112.19
2	F	5	NAG	O5-C1-C2	-2.09	107.98	111.29
2	G	7	MAN	C1-O5-C5	2.09	115.02	112.19
2	E	9	FUC	C1-O5-C5	2.06	117.45	112.78
2	E	4	MAN	C1-C2-C3	2.06	112.20	109.67
2	F	4	MAN	C1-O5-C5	2.06	114.98	112.19
2	G	5	NAG	C2-N2-C7	2.06	125.83	122.90
2	E	1	NAG	C1-C2-N2	-2.05	106.99	110.49
2	F	2	NAG	C1-O5-C5	2.03	114.95	112.19
2	E	8	NAG	C3-C4-C5	2.01	113.82	110.24
2	F	7	MAN	C1-O5-C5	2.00	114.91	112.19

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	2	NAG	O5-C5-C6-O6
2	G	5	NAG	C8-C7-N2-C2
2	E	8	NAG	O5-C5-C6-O6
2	G	7	MAN	O5-C5-C6-O6
2	G	5	NAG	O7-C7-N2-C2
2	G	5	NAG	C1-C2-N2-C7
2	G	2	NAG	C4-C5-C6-O6
2	G	5	NAG	O5-C5-C6-O6
2	G	5	NAG	C4-C5-C6-O6
2	H	7	MAN	O5-C5-C6-O6
2	E	7	MAN	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	G	7	MAN	C4-C5-C6-O6
2	E	8	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	4	MAN	C4-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6

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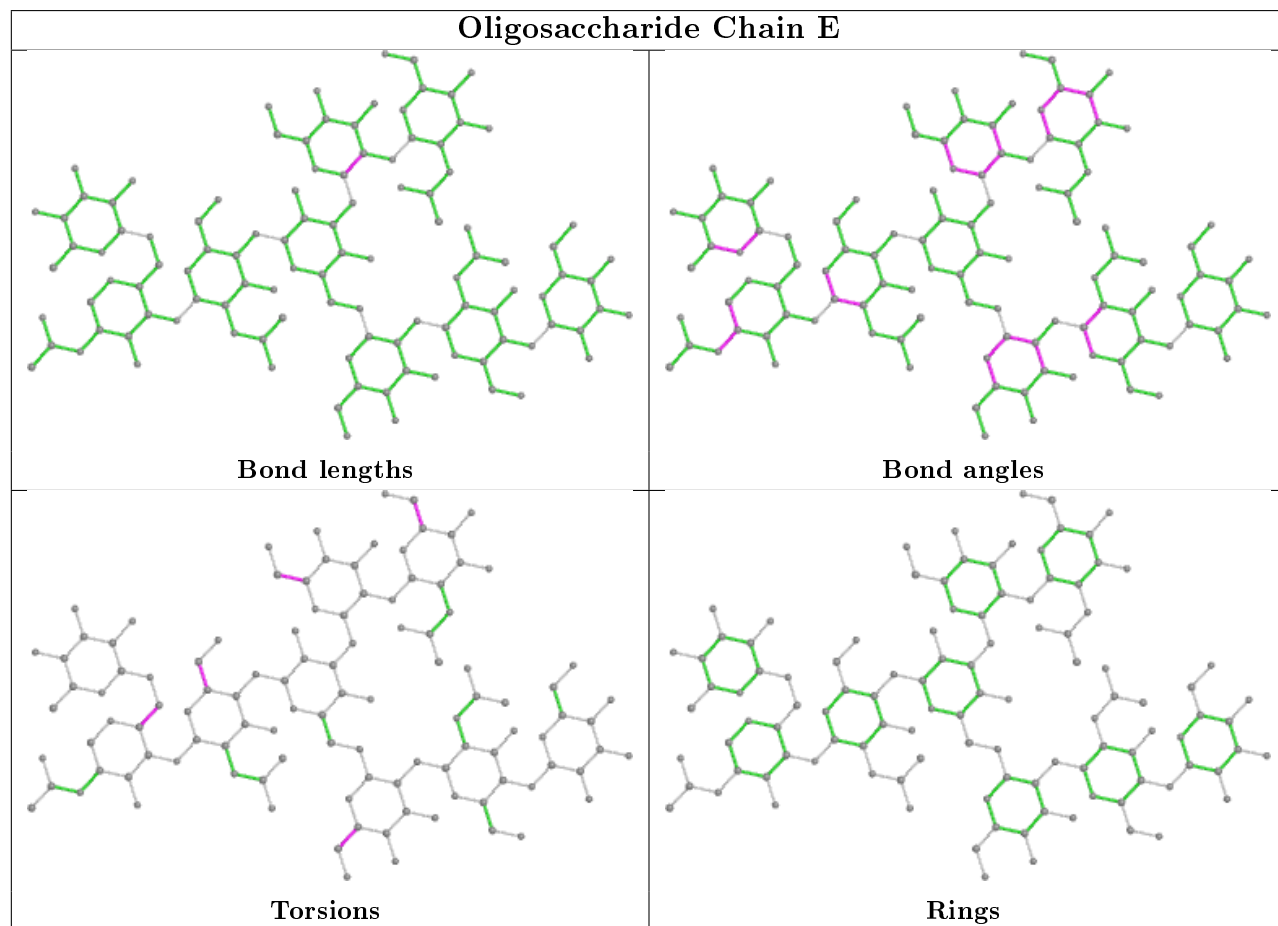
Mol	Chain	Res	Type	Atoms
2	H	3	BMA	O5-C5-C6-O6
2	G	8	NAG	C4-C5-C6-O6
2	F	4	MAN	C4-C5-C6-O6

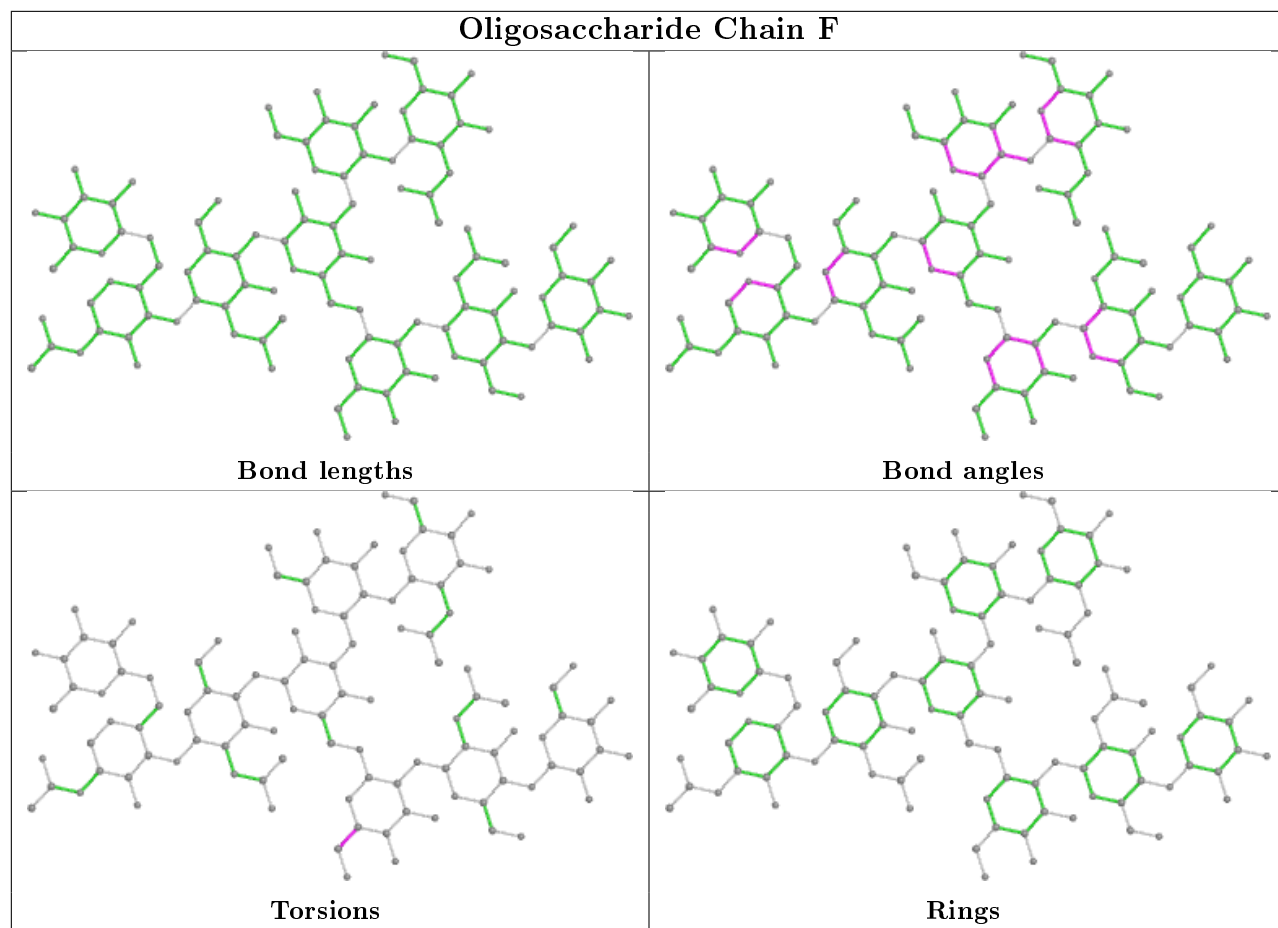
There are no ring outliers.

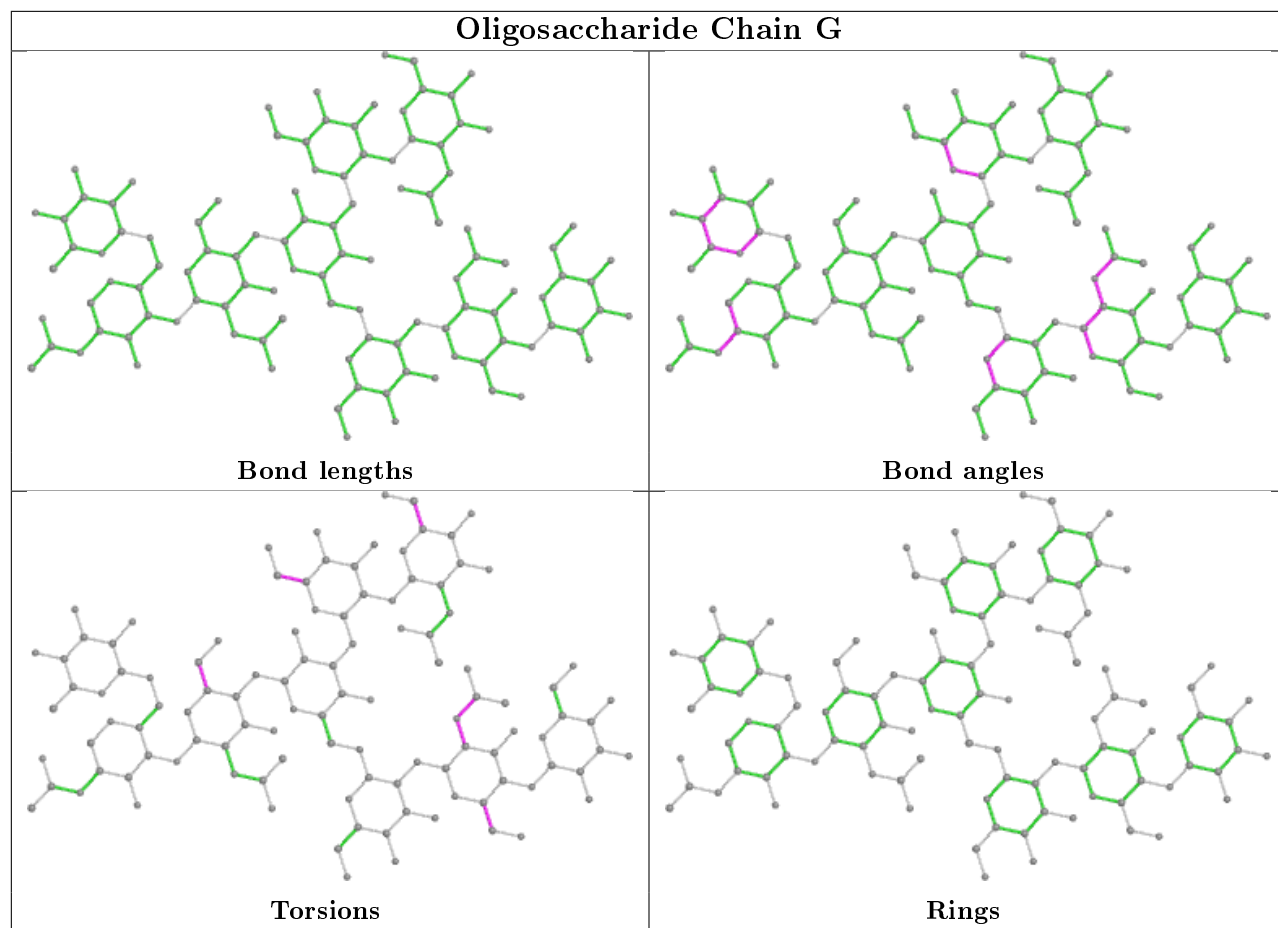
5 monomers are involved in 4 short contacts:

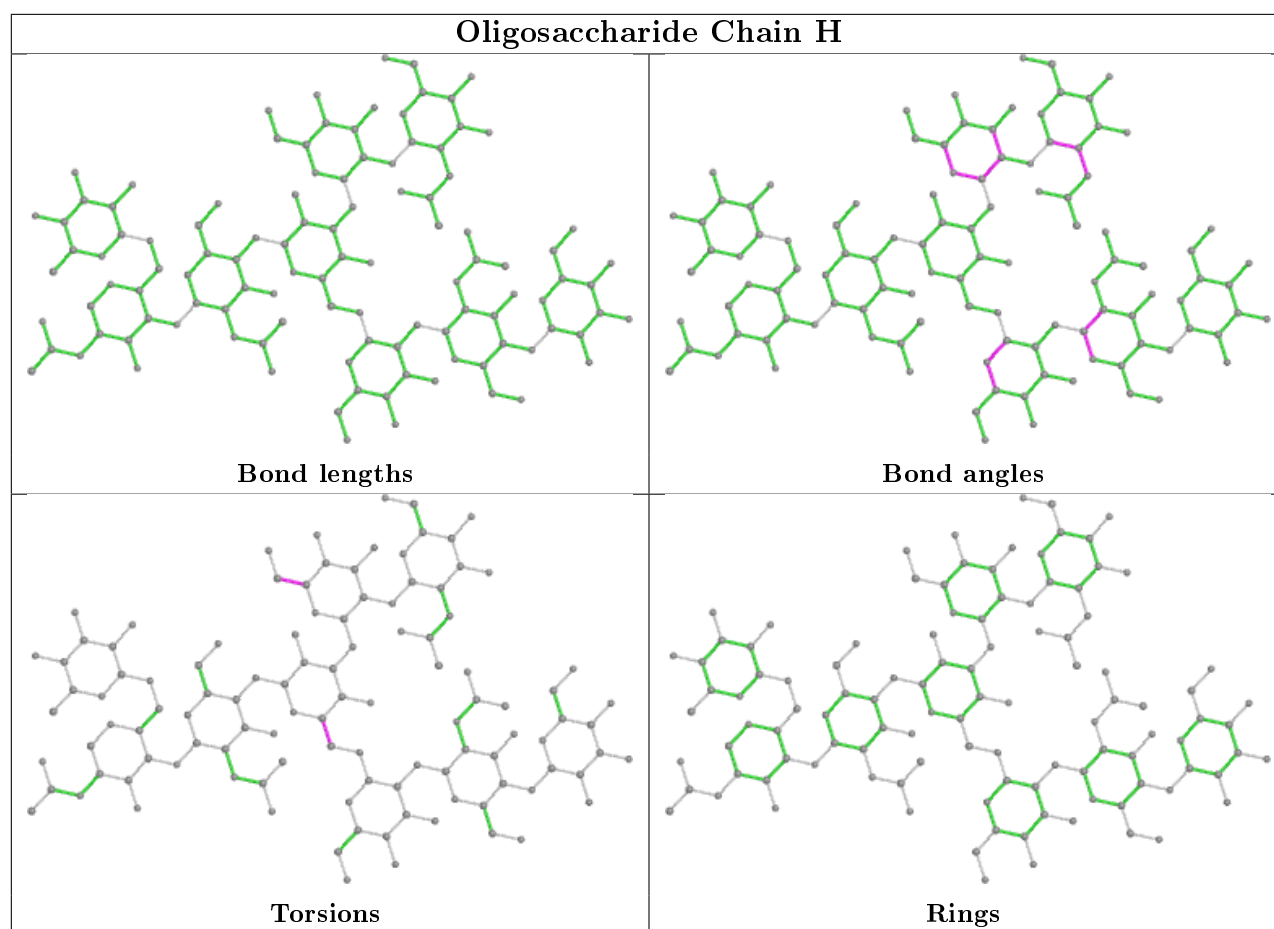
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	7	MAN	1	0
2	E	2	NAG	1	0
2	G	9	FUC	1	0
2	H	3	BMA	1	0
2	H	5	NAG	1	0

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](#)

There are no ligands in this entry.

## 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	209/227 (92%)	-0.11	0 100 100	59, 80, 110, 127	0
1	B	209/227 (92%)	0.29	7 (3%) 46 41	56, 97, 143, 166	0
1	C	208/227 (91%)	0.38	14 (6%) 17 13	60, 103, 163, 178	0
1	D	209/227 (92%)	-0.04	0 100 100	58, 81, 116, 137	0
All	All	835/908 (91%)	0.13	21 (2%) 57 55	56, 86, 145, 178	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	324	SER	5.4
1	B	310	HIS	5.3
1	C	275	PHE	5.1
1	C	276	ASN	4.3
1	C	277	TRP	4.2
1	B	296	TYR	3.6
1	C	239	SER	3.2
1	B	323	VAL	3.1
1	C	278	TYR	3.1
1	C	273	VAL	2.8
1	C	264	VAL	2.5
1	C	333	GLU	2.4
1	C	321	CYS	2.4
1	B	236	GLY	2.3
1	B	302	VAL	2.2
1	C	274	LYS	2.2
1	C	284	VAL	2.2
1	B	262	VAL	2.2
1	B	266	VAL	2.2
1	C	323	VAL	2.1
1	C	238	PRO	2.1



## 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	FUC	G	9	10/11	0.86	0.19	142,146,149,149	0
2	NAG	F	1	14/15	0.89	0.19	128,137,142,145	0
2	FUC	F	9	10/11	0.90	0.18	142,149,153,156	0
2	NAG	G	8	14/15	0.90	0.10	167,174,177,177	0
2	MAN	E	7	11/12	0.90	0.16	127,130,135,142	0
2	MAN	H	7	11/12	0.91	0.16	140,147,151,153	0
2	NAG	F	8	14/15	0.91	0.16	147,151,154,155	0
2	NAG	F	5	14/15	0.92	0.14	118,120,124,124	0
2	MAN	H	4	11/12	0.92	0.19	112,119,126,127	0
2	NAG	H	8	14/15	0.92	0.14	135,141,143,144	0
2	MAN	G	7	11/12	0.92	0.10	154,159,160,168	0
2	FUC	H	9	10/11	0.92	0.18	115,119,123,123	0
2	GAL	G	6	11/12	0.92	0.16	103,111,114,114	0
2	NAG	E	8	14/15	0.93	0.21	135,145,149,149	0
2	MAN	F	4	11/12	0.93	0.11	121,126,127,129	0
2	FUC	E	9	10/11	0.93	0.22	124,129,134,136	0
2	BMA	G	3	11/12	0.93	0.11	114,130,135,142	0
2	NAG	G	2	14/15	0.94	0.20	120,130,137,137	0
2	NAG	H	1	14/15	0.94	0.13	107,111,127,128	0
2	BMA	H	3	11/12	0.94	0.11	114,116,124,132	0
2	NAG	G	1	14/15	0.94	0.18	138,146,155,160	0
2	GAL	F	6	11/12	0.94	0.12	129,132,136,137	0
2	MAN	F	7	11/12	0.94	0.13	135,140,142,145	0
2	GAL	E	6	11/12	0.95	0.16	104,109,114,115	0
2	NAG	F	2	14/15	0.95	0.10	108,113,119,120	0
2	BMA	E	3	11/12	0.95	0.12	96,102,108,118	0
2	BMA	F	3	11/12	0.96	0.09	115,117,122,128	0
2	NAG	E	1	14/15	0.96	0.14	98,110,118,120	0
2	NAG	H	2	14/15	0.96	0.14	101,106,108,114	0
2	MAN	G	4	11/12	0.96	0.10	100,110,115,115	0
2	MAN	E	4	11/12	0.96	0.17	105,111,122,123	0
2	NAG	E	5	14/15	0.97	0.19	104,107,114,114	0

*Continued on next page...*

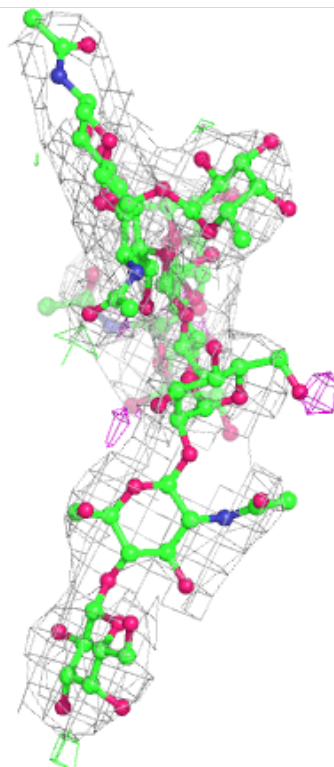
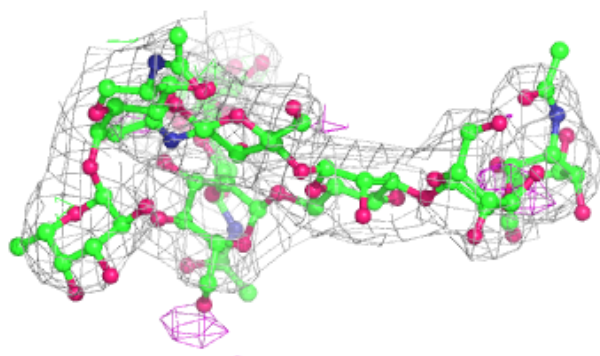
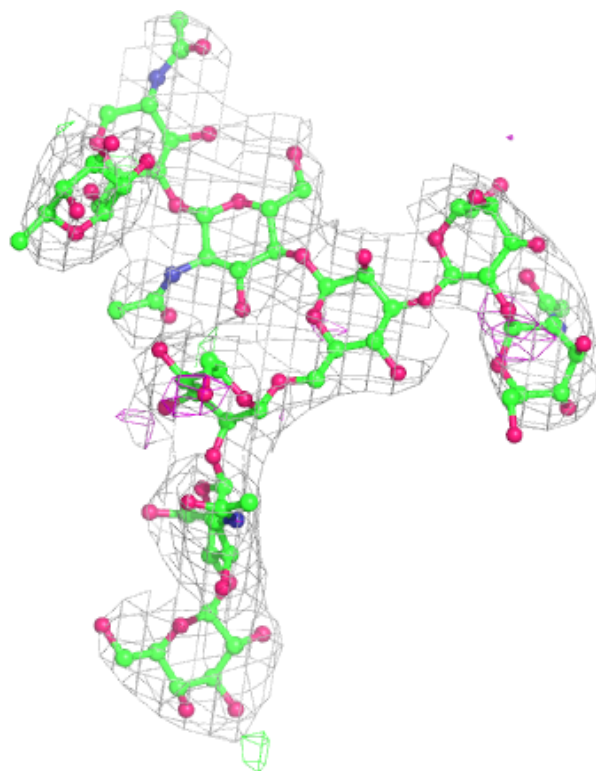
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	H	5	14/15	0.97	0.16	98,102,106,107	0
2	GAL	H	6	11/12	0.97	0.17	91,96,98,99	0
2	NAG	G	5	14/15	0.97	0.11	101,104,106,107	0
2	NAG	E	2	14/15	0.98	0.14	85,91,97,98	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.

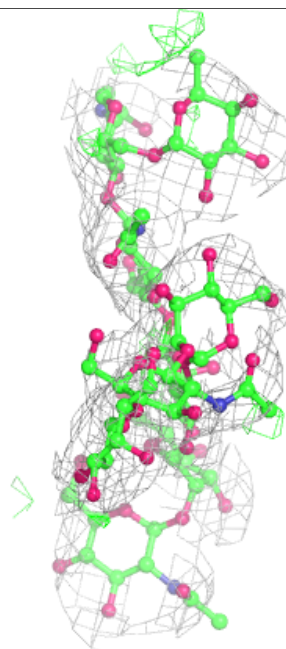
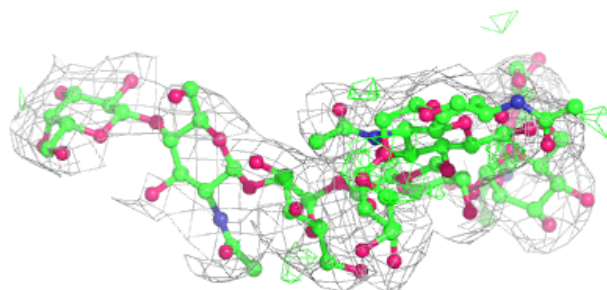
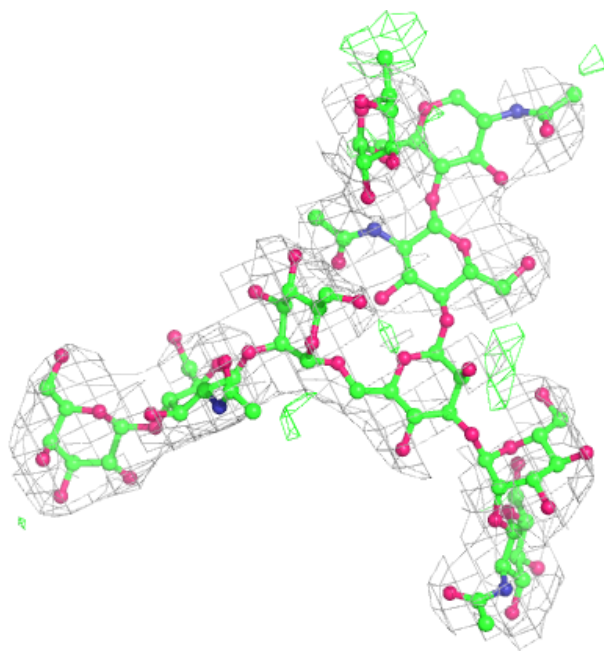
**Electron density around Chain E:**

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



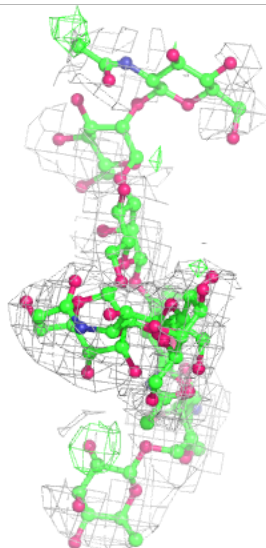
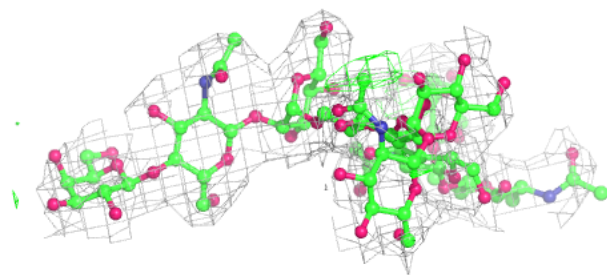
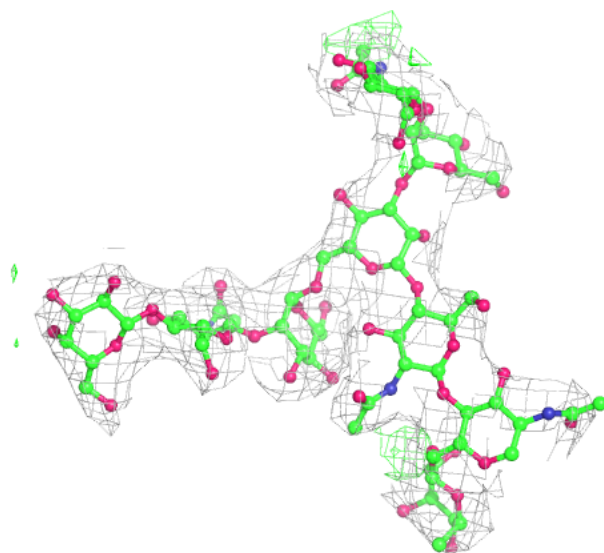
**Electron density around Chain F:**

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



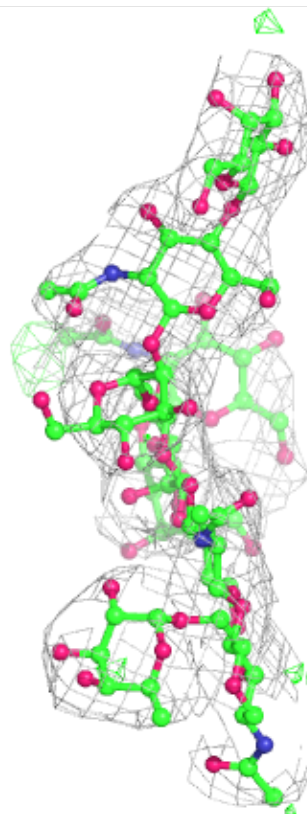
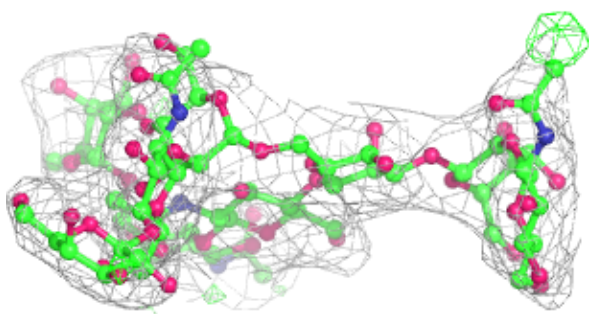
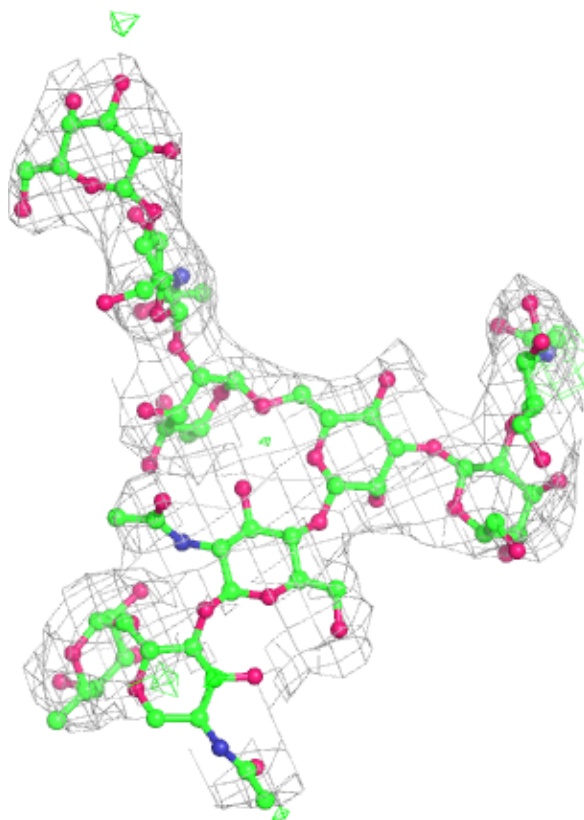
**Electron density around Chain G:**

$2mF_o-DF_c$  (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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.