



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2023 – 07:05 AM EDT

PDB ID : 3QHN  
Title : Crystal analysis of the complex structure, E201A-cellobiose, of endocellulase from *pyrococcus horikoshii*  
Authors : Kim, H.-W.; Ishikawa, K.  
Deposited on : 2011-01-26  
Resolution : 1.99 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

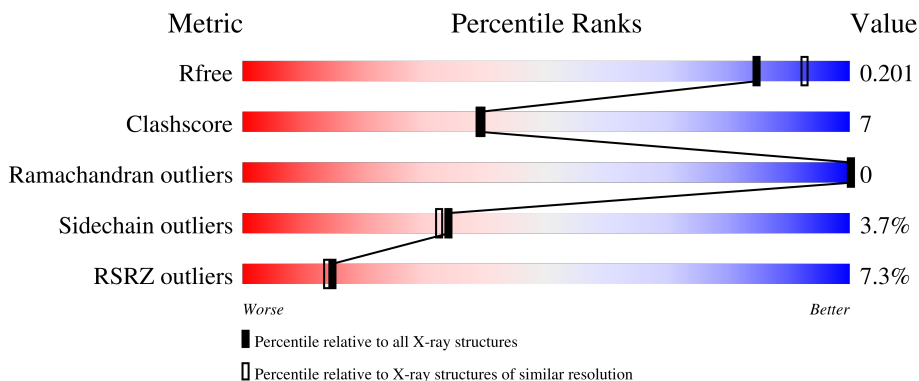
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	458	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-top: 5px;">5%      67%      14%      •      18%</p>
1	B	458	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-top: 5px;">2%      72%      9%      •      18%</p>
1	C	458	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-top: 5px;">11%      62%      19%      •      18%</p>
2	D	4	<div style="display: flex; align-items: center;"> <div style="width: 75%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="margin-top: 5px;">75%      25%</p>
2	E	4	<div style="display: flex; align-items: center;"> <div style="width: 50%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="margin-top: 5px;">50%      50%</p>

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Mol	Chain	Length	Quality of chain
2	G	4	 50% 50%
3	F	2	 50% 50%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9624 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 458aa long hypothetical endo-1,4-beta-glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	377	3067	2000	502	555	10	0	0	0
1	B	377	3067	2000	502	555	10	0	0	0
1	C	377	3067	2000	502	555	10	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	ALA	GLU	engineered mutation	UNP O58925
B	201	ALA	GLU	engineered mutation	UNP O58925
C	201	ALA	GLU	engineered mutation	UNP O58925

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	D	4	45	24	21	0	0	0
2	E	4	45	24	21	0	0	0
2	G	4	45	24	21	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	F	2	Total	C	O	0	0	0
			23	12	11			

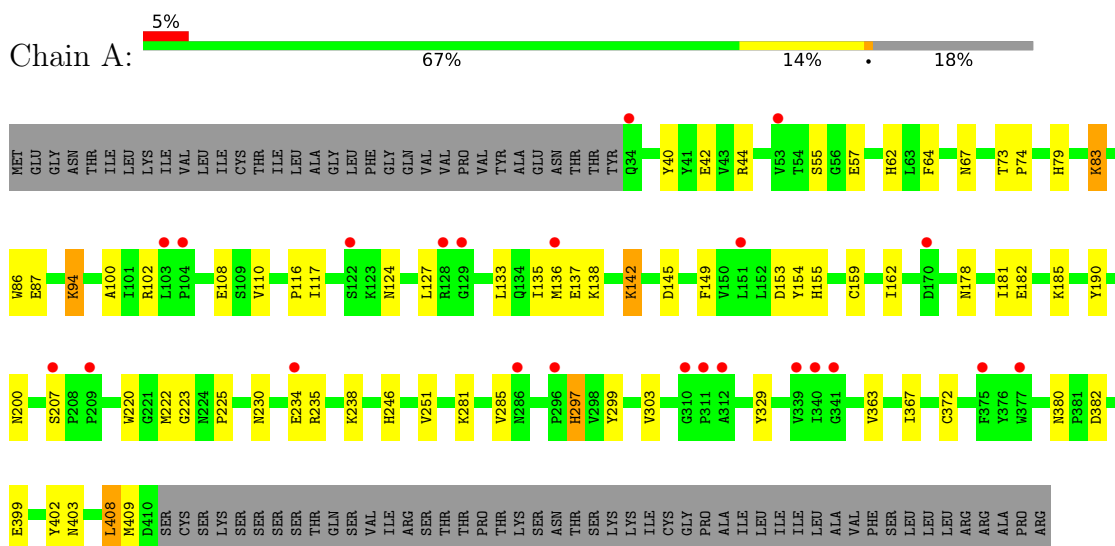
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		
4	B	106	Total	O	0	0
			106	106		
4	C	51	Total	O	0	0
			51	51		

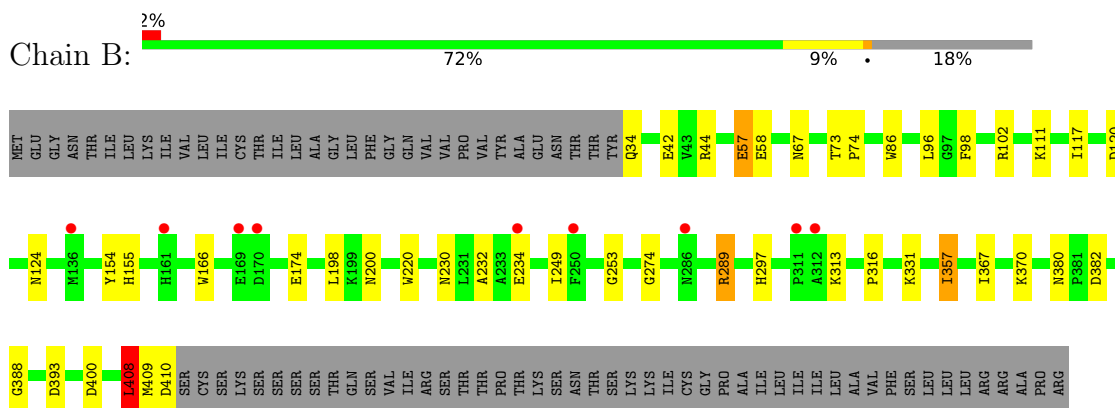
### 3 Residue-property plots

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.

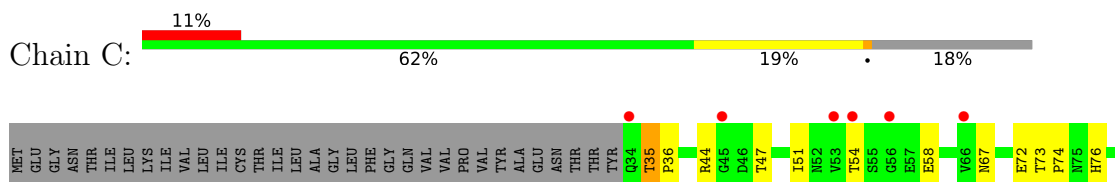
- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase

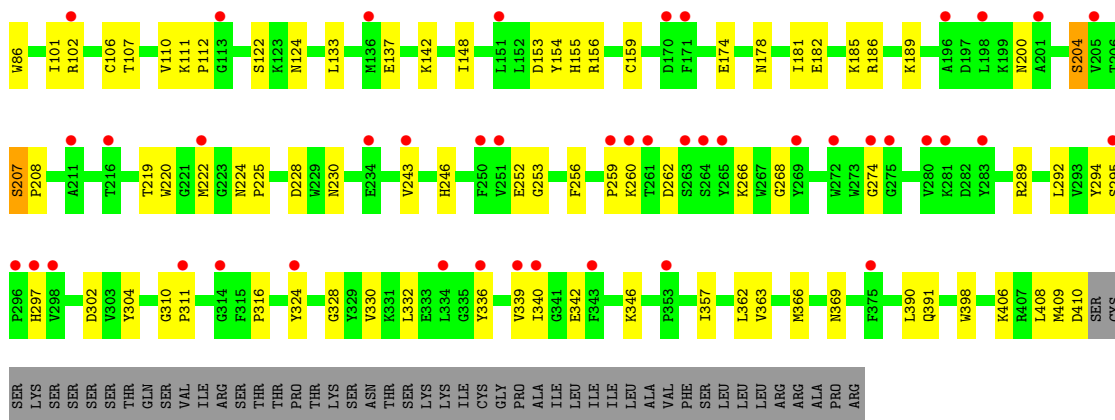


- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase



- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase





- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain D: 75% 25%

BCC1  
BCC2  
BCC3  
BCC4

- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain E: 50% 50%

BCC1  
BCC2  
BCC3  
BCC4

- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain G: 50% 50%

BCC1  
BCC2  
BCC3  
BCC4

- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain F: 50% 50%

BCC1  
BCC2

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.32Å 58.35Å 138.27Å 90.00° 109.61° 90.00°	Depositor
Resolution (Å)	28.99 – 1.99 28.99 – 1.99	Depositor EDS
% Data completeness (in resolution range)	94.8 (28.99-1.99) 90.8 (28.99-1.99)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.196 , 0.248 0.198 , 0.201	Depositor DCC
$R_{free}$ test set	3988 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtrriage
Anisotropy	0.436	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 52.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9624	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: BGC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.07	2/3178 (0.1%)	0.87	2/4339 (0.0%)
1	B	1.12	3/3178 (0.1%)	0.92	5/4339 (0.1%)
1	C	0.88	0/3178	0.80	1/4339 (0.0%)
All	All	1.03	5/9534 (0.1%)	0.87	8/13017 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	57	GLU	CG-CD	-6.25	1.42	1.51
1	B	98	PHE	CE1-CZ	5.64	1.48	1.37
1	A	402	TYR	CG-CD1	5.36	1.46	1.39
1	B	174	GLU	CG-CD	5.21	1.59	1.51
1	A	329	TYR	CE1-CZ	5.21	1.45	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	B	400	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	289	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	393	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	235	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	408	LEU	CA-CB-CG	5.40	127.71	115.30
1	A	153	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	390	LEU	CB-CG-CD1	-5.09	102.34	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	3067	0	2907	42	0
1	B	3067	0	2907	30	1
1	C	3067	0	2907	60	0
2	D	45	0	39	1	0
2	E	45	0	39	2	0
2	G	45	0	39	2	1
3	F	23	0	21	2	0
4	A	108	0	0	1	0
4	B	106	0	0	0	0
4	C	51	0	0	0	0
All	All	9624	0	8859	135	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (135) 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:316:PRO:HG3	1:B:357:ILE:CD1	1.87	1.04
1:B:316:PRO:HG3	1:B:357:ILE:HD13	1.53	0.89
1:C:266:LYS:HD2	1:C:266:LYS:H	1.34	0.89
1:B:67:ASN:HD21	1:B:102:ARG:HH11	1.24	0.86
1:C:67:ASN:HD21	1:C:102:ARG:HH11	1.29	0.80
1:C:35:THR:HB	1:C:246:HIS:HB3	1.68	0.76
1:C:181:ILE:HG22	1:C:185:LYS:HE3	1.69	0.74
1:A:67:ASN:HD21	1:A:102:ARG:HD3	1.51	0.72
1:A:55:SER:OG	1:A:57:GLU:HG3	1.90	0.72
1:C:266:LYS:H	1:C:266:LYS:CD	2.03	0.71
1:C:86:TRP:HD1	1:C:124:ASN:HD22	1.38	0.71
1:B:102:ARG:HH22	1:B:200:ASN:HD22	1.40	0.69
1:A:67:ASN:HD21	1:A:102:ARG:HH11	1.41	0.69
1:C:200:ASN:ND2	1:C:297:HIS:HE1	1.91	0.68
1:C:200:ASN:HD21	1:C:297:HIS:HE1	1.40	0.68
1:C:266:LYS:HD2	1:C:266:LYS:N	2.10	0.66
1:B:86:TRP:HD1	1:B:124:ASN:HD22	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:PRO:CG	1:B:357:ILE:CD1	2.71	0.65
1:A:133:LEU:O	1:A:137:GLU:HG3	1.97	0.64
1:B:102:ARG:HH22	1:B:200:ASN:ND2	1.95	0.64
1:B:67:ASN:ND2	1:B:102:ARG:HH11	1.95	0.64
1:B:316:PRO:HB3	1:B:357:ILE:HD11	1.80	0.64
1:B:331:LYS:HE3	1:B:370:LYS:O	1.98	0.63
1:C:362:LEU:O	1:C:366:MET:HG3	1.99	0.63
1:B:316:PRO:HG3	1:B:357:ILE:HD11	1.77	0.63
1:C:178:ASN:O	1:C:182:GLU:HG3	1.98	0.63
1:C:107:THR:HG22	1:C:111:LYS:HE3	1.81	0.62
1:A:83:LYS:O	1:A:83:LYS:HD3	1.99	0.62
1:C:102:ARG:HH22	1:C:200:ASN:HD22	1.49	0.61
1:C:342:GLU:OE1	2:G:1:BGC:H1	2.00	0.60
1:C:67:ASN:ND2	1:C:102:ARG:HH11	1.97	0.60
1:C:110:VAL:HA	1:C:133:LEU:HD13	1.83	0.60
1:C:137:GLU:OE2	1:C:186:ARG:HD3	2.03	0.58
1:A:116:PRO:O	1:A:117:ILE:HD13	2.03	0.58
1:C:302:ASP:OD2	1:C:346:LYS:HB2	2.04	0.57
1:A:299:TYR:CD1	1:A:303:VAL:HG21	2.39	0.57
1:C:406:LYS:HA	1:C:409:MET:CE	2.35	0.56
1:C:292:LEU:HD21	1:C:294:TYR:CZ	2.39	0.56
1:B:316:PRO:CG	1:B:357:ILE:HD11	2.34	0.56
1:C:406:LYS:HA	1:C:409:MET:HE3	1.88	0.56
1:A:102:ARG:HH22	1:A:200:ASN:HD22	1.54	0.55
1:C:204:SER:HG	1:C:256:PHE:HD2	1.53	0.55
1:A:363:VAL:HG13	1:A:408:LEU:HD13	1.88	0.55
1:C:324:TYR:HA	1:C:328:GLY:HA3	1.89	0.54
1:A:155:HIS:HA	1:A:200:ASN:CB	2.38	0.52
1:A:67:ASN:ND2	1:A:102:ARG:HH11	2.06	0.52
1:B:253:GLY:O	1:B:274:GLY:HA2	2.09	0.52
1:C:72:GLU:O	1:C:156:ARG:HD2	2.09	0.52
1:A:297:HIS:ND1	4:A:565:HOH:O	2.24	0.51
1:A:380:ASN:HB3	1:A:382:ASP:OD1	2.11	0.51
1:A:155:HIS:HA	1:A:200:ASN:HB3	1.93	0.51
1:C:102:ARG:HH22	1:C:200:ASN:ND2	2.09	0.50
1:B:380:ASN:HB3	1:B:382:ASP:OD1	2.11	0.50
1:C:86:TRP:HD1	1:C:124:ASN:ND2	2.09	0.50
3:F:2:BGC:O4	2:G:1:BGC:H6C1	2.11	0.50
1:B:316:PRO:CB	1:B:357:ILE:HD11	2.40	0.50
1:B:220:TRP:CE2	1:B:230:ASN:HB3	2.46	0.50
1:A:223:GLY:O	1:A:225:PRO:HD3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:HIS:CD2	1:A:372:CYS:SG	3.06	0.49
1:C:207:SER:HB3	1:C:208:PRO:HD2	1.93	0.49
1:B:230:ASN:O	1:B:234:GLU:HG3	2.12	0.49
1:C:252:GLU:HA	1:C:295:SER:O	2.12	0.49
1:C:316:PRO:HG3	1:C:357:ILE:CG2	2.42	0.49
1:C:391:GLN:HG2	1:C:398:TRP:CE2	2.47	0.49
1:C:106:CYS:HA	1:C:156:ARG:O	2.13	0.48
1:B:367:ILE:HG13	1:B:408:LEU:CD1	2.44	0.48
1:A:162:ILE:HD11	2:D:3:BGC:H2	1.94	0.48
1:A:110:VAL:HA	1:A:133:LEU:HD13	1.95	0.48
1:C:51:ILE:HG12	1:C:58:GLU:HB2	1.96	0.47
1:C:406:LYS:O	1:C:410:ASP:N	2.47	0.47
1:A:73:THR:HB	1:A:74:PRO:HD2	1.97	0.47
1:A:94:LYS:O	1:A:94:LYS:HE3	2.15	0.47
1:C:222:MET:SD	1:C:259:PRO:HD3	2.55	0.47
1:B:155:HIS:HA	1:B:200:ASN:HB3	1.97	0.47
2:E:3:BGC:H6C1	2:E:4:BGC:C1	2.44	0.47
1:B:102:ARG:NH2	1:B:200:ASN:HD22	2.12	0.47
1:C:224:ASN:HA	1:C:225:PRO:HD2	1.61	0.46
1:C:101:ILE:HD12	1:C:148:ILE:HG21	1.97	0.46
1:B:380:ASN:O	1:B:388:GLY:HA3	2.15	0.46
1:A:102:ARG:HH22	1:A:200:ASN:ND2	2.13	0.46
1:B:367:ILE:HG13	1:B:408:LEU:HD13	1.97	0.46
1:C:310:GLY:O	1:C:311:PRO:C	2.52	0.46
1:C:86:TRP:H	1:C:124:ASN:HD21	1.62	0.45
1:C:67:ASN:HD21	1:C:102:ARG:HD3	1.80	0.45
1:A:251:VAL:HG11	1:A:285:VAL:HG21	1.98	0.45
1:A:367:ILE:HG13	1:A:408:LEU:CD1	2.47	0.45
1:C:36:PRO:HD2	1:C:246:HIS:CE1	2.51	0.45
1:C:219:THR:O	1:C:228:ASP:HA	2.16	0.45
1:B:198:LEU:HD21	1:B:249:ILE:HG23	1.99	0.45
1:A:40:TYR:HA	1:A:246:HIS:HB2	1.99	0.45
1:C:44:ARG:NH1	1:C:58:GLU:OE1	2.47	0.44
1:C:228:ASP:HB3	1:C:230:ASN:OD1	2.17	0.44
2:E:3:BGC:H6C1	2:E:4:BGC:O2	2.17	0.44
1:A:87:GLU:CD	1:A:142:LYS:HE3	2.37	0.44
1:C:142:LYS:HA	1:C:142:LYS:HD3	1.84	0.44
1:A:178:ASN:O	1:A:182:GLU:HG3	2.18	0.44
1:A:67:ASN:ND2	1:A:102:ARG:HD3	2.28	0.44
1:A:142:LYS:O	1:A:145:ASP:HB2	2.18	0.43
1:C:44:ARG:HH12	1:C:58:GLU:CD	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLU:OE1	1:A:44:ARG:CZ	2.66	0.43
1:A:155:HIS:HA	1:A:200:ASN:HB2	2.01	0.43
1:A:64:PHE:CD2	1:A:409:MET:HG2	2.53	0.43
1:C:262:ASP:O	1:C:268:GLY:HA3	2.18	0.43
1:C:330:VAL:HG12	1:C:336:TYR:HB2	2.00	0.43
1:B:200:ASN:ND2	1:B:297:HIS:HE1	2.17	0.43
1:A:220:TRP:CE2	1:A:230:ASN:HB3	2.53	0.43
1:C:253:GLY:O	1:C:274:GLY:HA2	2.18	0.43
1:C:304:TYR:CD1	3:F:1:BGC:H5	2.54	0.43
1:A:181:ILE:O	1:A:185:LYS:HG3	2.19	0.42
1:C:220:TRP:NE1	1:C:230:ASN:HB3	2.34	0.42
1:A:127:LEU:HD22	1:A:135:ILE:HG12	2.00	0.42
1:B:57:GLU:HG3	1:B:58:GLU:N	2.34	0.42
1:C:295:SER:HA	1:C:339:VAL:O	2.19	0.42
1:B:96:LEU:O	1:B:409:MET:HE1	2.19	0.42
1:C:73:THR:HB	1:C:74:PRO:CD	2.49	0.42
1:C:363:VAL:HG13	1:C:408:LEU:HB2	2.01	0.42
1:A:79:HIS:HB2	1:A:380:ASN:ND2	2.35	0.42
1:C:58:GLU:O	1:C:58:GLU:HG2	2.18	0.42
1:C:155:HIS:HA	1:C:200:ASN:HB3	2.00	0.42
1:C:181:ILE:CG2	1:C:185:LYS:HE3	2.46	0.42
1:A:190:TYR:CD2	1:A:190:TYR:N	2.87	0.42
1:A:86:TRP:HD1	1:A:124:ASN:ND2	2.18	0.42
1:C:220:TRP:CE2	1:C:230:ASN:HB3	2.54	0.41
1:C:406:LYS:HG3	1:C:409:MET:HE3	2.02	0.41
1:A:100:ALA:HA	1:A:149:PHE:O	2.20	0.41
1:A:142:LYS:HA	1:A:142:LYS:HD3	1.96	0.41
1:A:234:GLU:O	1:A:238:LYS:HG3	2.21	0.41
1:B:370:LYS:HB2	1:B:370:LYS:HE3	1.89	0.41
1:A:108:GLU:HB2	1:A:159:CYS:SG	2.61	0.41
1:B:120:ASP:OD1	1:B:120:ASP:C	2.60	0.41
1:A:281:LYS:HE2	1:A:281:LYS:HB3	1.72	0.40
1:C:76:HIS:HE1	1:C:159:CYS:SG	2.43	0.40
1:C:332:LEU:HD21	1:C:369:ASN:HB3	2.03	0.40
1:B:166:TRP:CZ2	1:B:232:ALA:HB2	2.56	0.40
1:B:73:THR:HB	1:B:74:PRO:CD	2.51	0.40

All (1) 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)
1:B:42:GLU:OE2	2:G:4:BGC:O4[4_545]	2.15	0.05

### 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	375/458 (82%)	362 (96%)	13 (4%)	0	100	100
1	B	375/458 (82%)	365 (97%)	10 (3%)	0	100	100
1	C	375/458 (82%)	361 (96%)	14 (4%)	0	100	100
All	All	1125/1374 (82%)	1088 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	323/395 (82%)	311 (96%)	12 (4%)	34	32
1	B	323/395 (82%)	314 (97%)	9 (3%)	43	44
1	C	323/395 (82%)	308 (95%)	15 (5%)	27	23
All	All	969/1185 (82%)	933 (96%)	36 (4%)	34	32

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	LYS
1	A	94	LYS
1	A	136	MET
1	A	138	LYS
1	A	142	LYS
1	A	154	TYR
1	A	207	SER
1	A	222	MET
1	A	297	HIS
1	A	399	GLU
1	A	403	ASN
1	A	408	LEU
1	B	34	GLN
1	B	111	LYS
1	B	117	ILE
1	B	154	TYR
1	B	289	ARG
1	B	313	LYS
1	B	357	ILE
1	B	408	LEU
1	B	410	ASP
1	C	35	THR
1	C	47	THR
1	C	54	THR
1	C	112	PRO
1	C	122	SER
1	C	153	ASP
1	C	154	TYR
1	C	174	GLU
1	C	189	LYS
1	C	204	SER
1	C	207	SER
1	C	243	VAL
1	C	260	LYS
1	C	289	ARG
1	C	340	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	67	ASN
1	A	124	ASN

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Mol	Chain	Res	Type
1	A	200	ASN
1	A	359	GLN
1	B	34	GLN
1	B	67	ASN
1	B	124	ASN
1	B	161	HIS
1	B	200	ASN
1	B	359	GLN
1	C	34	GLN
1	C	67	ASN
1	C	76	HIS
1	C	115	GLN
1	C	124	ASN
1	C	161	HIS
1	C	200	ASN
1	C	297	HIS
1	C	359	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

14 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	BGC	D	1	2	12,12,12	1.05	1 (8%)	17,17,17	1.29	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BGC	D	2	2	11,11,12	1.15	1 (9%)	15,15,17	1.66	5 (33%)
2	BGC	D	3	2	11,11,12	2.66	4 (36%)	15,15,17	2.41	6 (40%)
2	BGC	D	4	2	11,11,12	1.32	1 (9%)	15,15,17	1.30	1 (6%)
2	BGC	E	1	2	12,12,12	1.67	3 (25%)	17,17,17	1.61	3 (17%)
2	BGC	E	2	2	11,11,12	1.35	1 (9%)	15,15,17	1.53	3 (20%)
2	BGC	E	3	2	11,11,12	1.67	3 (27%)	15,15,17	2.54	8 (53%)
2	BGC	E	4	2	11,11,12	0.94	1 (9%)	15,15,17	1.00	1 (6%)
3	BGC	F	1	3	12,12,12	0.54	0	17,17,17	0.86	1 (5%)
3	BGC	F	2	3	11,11,12	0.55	0	15,15,17	0.87	0
2	BGC	G	1	2	12,12,12	1.44	2 (16%)	17,17,17	2.34	7 (41%)
2	BGC	G	2	2	11,11,12	0.93	1 (9%)	15,15,17	1.49	3 (20%)
2	BGC	G	3	2	11,11,12	0.99	2 (18%)	15,15,17	1.86	3 (20%)
2	BGC	G	4	2	11,11,12	1.37	2 (18%)	15,15,17	2.34	4 (26%)

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	BGC	D	1	2	-	0/2/22/22	0/1/1/1
2	BGC	D	2	2	-	1/2/19/22	0/1/1/1
2	BGC	D	3	2	-	0/2/19/22	0/1/1/1
2	BGC	D	4	2	-	0/2/19/22	0/1/1/1
2	BGC	E	1	2	-	2/2/22/22	0/1/1/1
2	BGC	E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	E	3	2	-	2/2/19/22	0/1/1/1
2	BGC	E	4	2	-	1/2/19/22	0/1/1/1
3	BGC	F	1	3	-	0/2/22/22	0/1/1/1
3	BGC	F	2	3	-	0/2/19/22	0/1/1/1
2	BGC	G	1	2	-	2/2/22/22	0/1/1/1
2	BGC	G	2	2	-	0/2/19/22	0/1/1/1
2	BGC	G	3	2	-	1/2/19/22	0/1/1/1
2	BGC	G	4	2	-	0/2/19/22	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	BGC	O5-C1	6.54	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	BGC	O5-C1	4.08	1.50	1.43
2	E	3	BGC	O5-C1	3.66	1.49	1.43
2	G	1	BGC	O5-C1	3.16	1.50	1.42
2	D	3	BGC	C2-C3	3.16	1.57	1.52
2	D	4	BGC	O5-C1	3.06	1.48	1.43
2	D	3	BGC	O5-C5	2.93	1.49	1.43
2	D	2	BGC	O5-C5	2.90	1.49	1.43
2	E	1	BGC	O1-C1	2.87	1.48	1.39
2	E	3	BGC	C6-C5	2.68	1.60	1.51
2	E	1	BGC	O4-C4	2.59	1.49	1.43
2	G	1	BGC	O1-C1	2.49	1.47	1.39
2	G	4	BGC	C4-C5	2.45	1.58	1.53
2	D	3	BGC	O2-C2	2.36	1.48	1.43
2	D	1	BGC	O4-C4	2.35	1.48	1.43
2	G	4	BGC	C4-C3	2.26	1.58	1.52
2	G	3	BGC	O5-C5	2.20	1.47	1.43
2	E	4	BGC	O5-C5	2.19	1.47	1.43
2	E	1	BGC	C1-C2	2.17	1.57	1.52
2	G	3	BGC	O5-C1	2.14	1.47	1.43
2	E	3	BGC	C4-C5	2.09	1.57	1.53
2	G	2	BGC	O5-C1	2.03	1.47	1.43

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	BGC	C1-O5-C5	6.49	120.99	112.19
2	G	3	BGC	O4-C4-C3	-5.82	96.90	110.35
2	G	1	BGC	C6-C5-C4	-5.77	99.49	113.00
2	G	4	BGC	C1-O5-C5	-4.85	105.62	112.19
2	E	3	BGC	C3-C4-C5	4.60	118.45	110.24
2	G	4	BGC	C6-C5-C4	4.60	123.77	113.00
2	G	4	BGC	O5-C1-C2	4.56	117.81	110.77
2	E	3	BGC	O5-C1-C2	4.32	117.43	110.77
2	E	3	BGC	O3-C3-C2	-4.18	101.98	109.99
2	G	1	BGC	O4-C4-C3	3.94	119.47	110.35
2	D	3	BGC	C3-C4-C5	-3.84	103.39	110.24
2	G	2	BGC	C1-O5-C5	3.75	117.27	112.19
2	D	4	BGC	O5-C5-C6	-3.47	101.76	107.20
2	E	2	BGC	C1-C2-C3	-3.42	105.46	109.67
2	G	1	BGC	C1-O5-C5	3.33	119.95	113.66
2	D	3	BGC	O2-C2-C3	3.21	116.58	110.14
2	E	3	BGC	C1-O5-C5	-3.11	107.98	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	BGC	O5-C1-C2	-2.79	105.30	110.28
2	E	3	BGC	C1-C2-C3	2.78	113.08	109.67
2	D	2	BGC	O3-C3-C2	2.77	115.29	109.99
2	G	2	BGC	O4-C4-C5	-2.73	102.51	109.30
2	D	2	BGC	O5-C1-C2	-2.72	106.56	110.77
2	G	1	BGC	C3-C4-C5	-2.72	105.39	110.24
2	G	2	BGC	O5-C5-C6	2.71	111.46	107.20
2	D	2	BGC	O2-C2-C1	-2.70	103.62	109.15
2	G	1	BGC	C1-C2-C3	2.70	115.91	110.31
2	E	1	BGC	O3-C3-C4	-2.61	104.32	110.35
2	E	1	BGC	O5-C5-C4	2.52	114.28	109.69
2	E	3	BGC	O2-C2-C3	-2.45	105.22	110.14
2	G	4	BGC	O5-C5-C4	-2.45	104.87	110.83
2	D	3	BGC	C6-C5-C4	2.34	118.49	113.00
2	D	2	BGC	O4-C4-C3	-2.34	104.94	110.35
2	E	4	BGC	O3-C3-C2	-2.30	105.59	109.99
2	G	3	BGC	O5-C5-C6	2.28	110.78	107.20
2	D	2	BGC	O5-C5-C6	2.28	110.78	107.20
3	F	1	BGC	C1-O5-C5	-2.26	109.40	113.66
2	G	1	BGC	O5-C5-C4	2.24	113.76	109.69
2	E	3	BGC	C2-C3-C4	-2.23	107.03	110.89
2	E	3	BGC	O5-C5-C6	-2.22	103.72	107.20
2	D	3	BGC	O4-C4-C5	-2.22	103.80	109.30
2	E	2	BGC	O5-C1-C2	-2.21	107.36	110.77
2	E	2	BGC	O4-C4-C5	-2.18	103.90	109.30
2	G	3	BGC	C1-C2-C3	-2.08	107.11	109.67
2	D	3	BGC	O5-C1-C2	2.07	113.97	110.77
2	G	1	BGC	O4-C4-C5	-2.03	104.26	109.30

There are no chirality outliers.

All (9) torsion outliers are listed below:

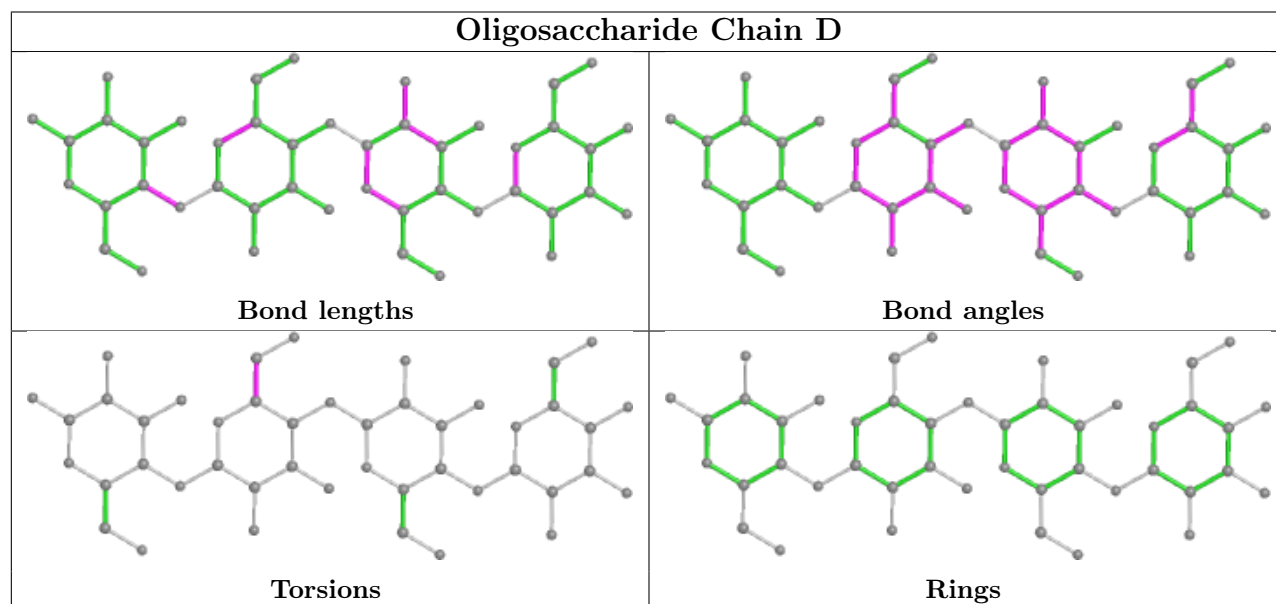
Mol	Chain	Res	Type	Atoms
2	E	1	BGC	O5-C5-C6-O6
2	E	1	BGC	C4-C5-C6-O6
2	G	1	BGC	C4-C5-C6-O6
2	G	1	BGC	O5-C5-C6-O6
2	G	3	BGC	O5-C5-C6-O6
2	E	3	BGC	C4-C5-C6-O6
2	E	3	BGC	O5-C5-C6-O6
2	D	2	BGC	O5-C5-C6-O6
2	E	4	BGC	O5-C5-C6-O6

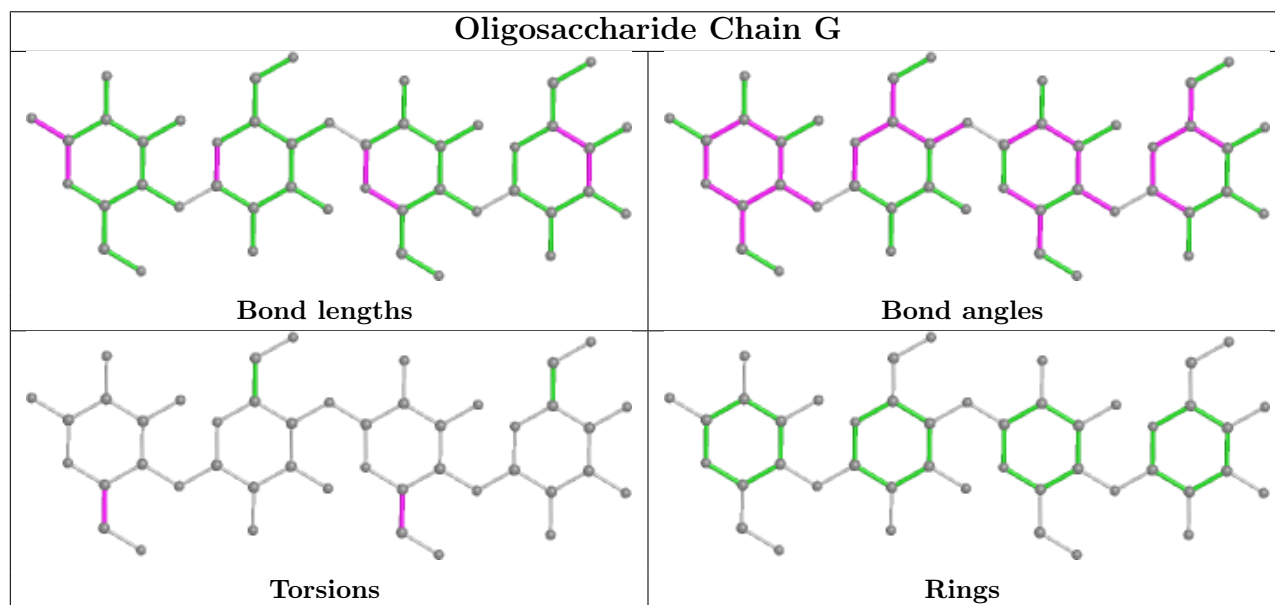
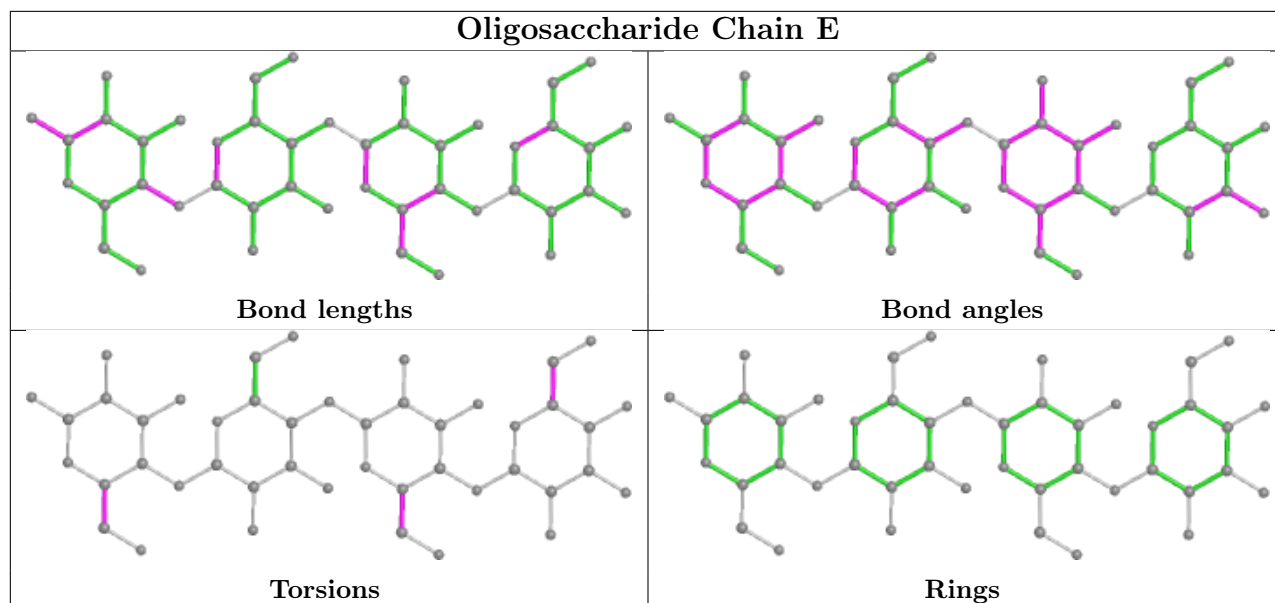
There are no ring outliers.

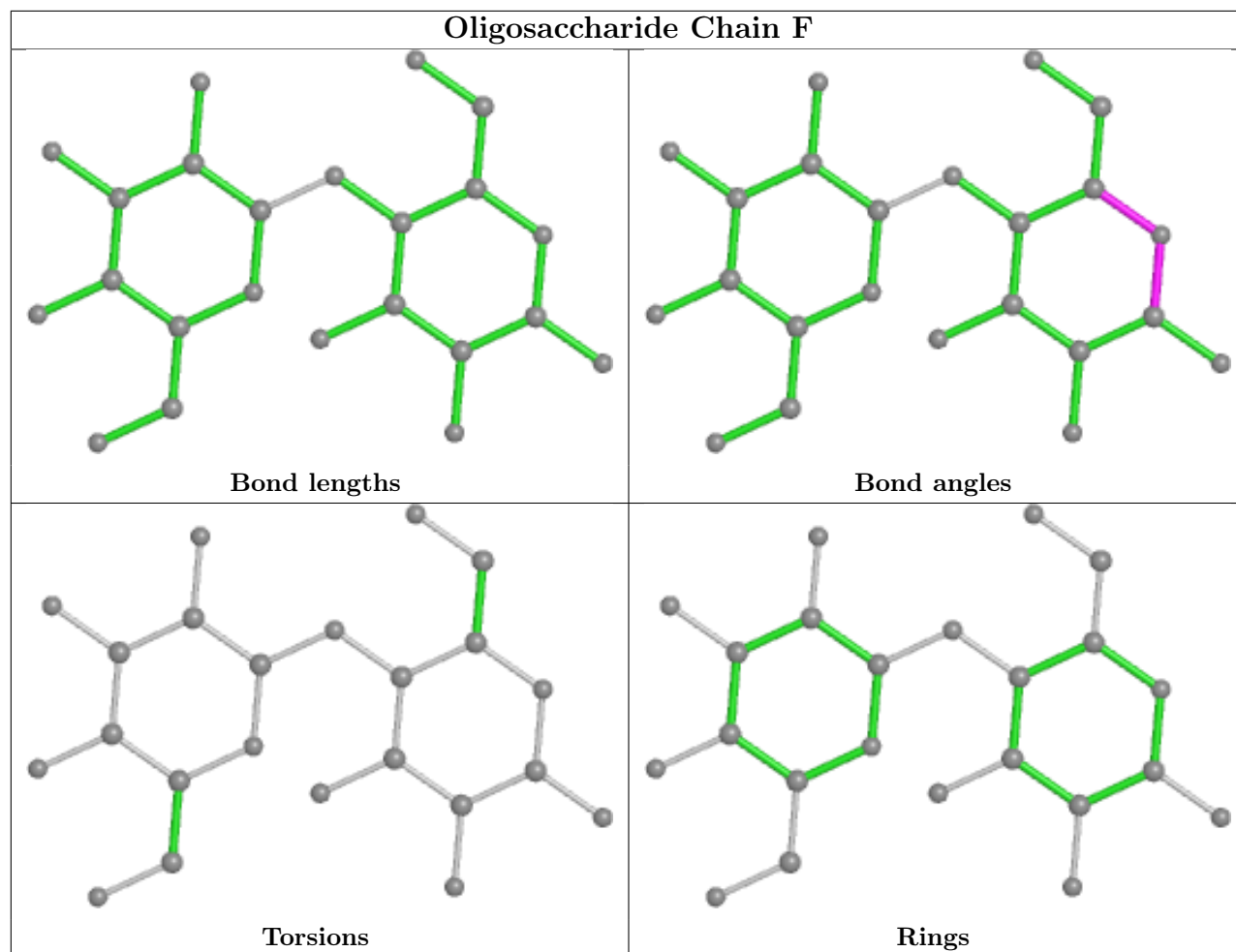
7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	BGC	2	0
3	F	1	BGC	1	0
2	D	3	BGC	1	0
2	E	3	BGC	2	0
3	F	2	BGC	1	0
2	G	4	BGC	0	1
2	E	4	BGC	2	0

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







## 5.6 Ligand geometry [i](#)

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	377/458 (82%)	0.23	23 (6%) 21 20	13, 25, 49, 56	8 (2%)
1	B	377/458 (82%)	0.05	9 (2%) 59 57	11, 22, 36, 46	10 (2%)
1	C	377/458 (82%)	0.76	50 (13%) 3 2	19, 38, 57, 64	9 (2%)
All	All	1131/1374 (82%)	0.35	82 (7%) 15 14	11, 27, 53, 64	27 (2%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	MET	6.9
1	C	136	MET	6.6
1	B	136	MET	5.6
1	C	340	ILE	4.9
1	C	54	THR	4.7
1	C	53	VAL	4.4
1	A	311	PRO	4.3
1	C	216	THR	4.2
1	A	209	PRO	4.2
1	C	283	TYR	4.1
1	C	205	VAL	4.0
1	B	169	GLU	4.0
1	C	260	LYS	4.0
1	C	334	LEU	4.0
1	C	296	PRO	3.9
1	A	122	SER	3.9
1	C	324	TYR	3.8
1	C	314	GLY	3.5
1	C	375	PHE	3.5
1	C	34	GLN	3.5
1	C	251	VAL	3.4
1	C	339	VAL	3.4
1	C	298	VAL	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	263	SER	3.3
1	C	280	VAL	3.2
1	C	261	THR	3.2
1	B	170	ASP	3.2
1	C	151	LEU	3.2
1	A	286	ASN	3.2
1	A	128	ARG	3.1
1	C	275	GLY	3.0
1	C	45	GLY	2.9
1	C	234	GLU	2.9
1	C	243	VAL	2.9
1	B	161	HIS	2.9
1	A	53	VAL	2.9
1	B	234	GLU	2.9
1	C	196	ALA	2.8
1	A	310	GLY	2.7
1	B	311	PRO	2.7
1	C	264	SER	2.7
1	A	375	PHE	2.7
1	A	377	TRP	2.7
1	C	198	LEU	2.7
1	C	201	ALA	2.7
1	C	336	TYR	2.7
1	B	312	ALA	2.6
1	C	259	PRO	2.6
1	A	234	GLU	2.6
1	C	56	GLY	2.6
1	C	353	PRO	2.5
1	A	341	GLY	2.5
1	A	340	ILE	2.5
1	C	295	SER	2.5
1	C	171	PHE	2.5
1	C	113	GLY	2.5
1	A	207	SER	2.5
1	C	265	TYR	2.4
1	A	312	ALA	2.4
1	A	296	PRO	2.4
1	C	250	PHE	2.4
1	C	311	PRO	2.4
1	C	343	PHE	2.3
1	A	151	LEU	2.3
1	A	34	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	170	ASP	2.3
1	C	269	TYR	2.3
1	A	170	ASP	2.3
1	C	297	HIS	2.2
1	C	274	GLY	2.2
1	B	250	PHE	2.2
1	B	286	ASN	2.2
1	C	211	ALA	2.2
1	C	272	TRP	2.1
1	C	222	MET	2.1
1	C	102	ARG	2.1
1	C	281	LYS	2.1
1	A	129	GLY	2.1
1	A	103	LEU	2.1
1	A	104	PRO	2.1
1	A	339	VAL	2.0
1	C	66	VAL	2.0

## 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.

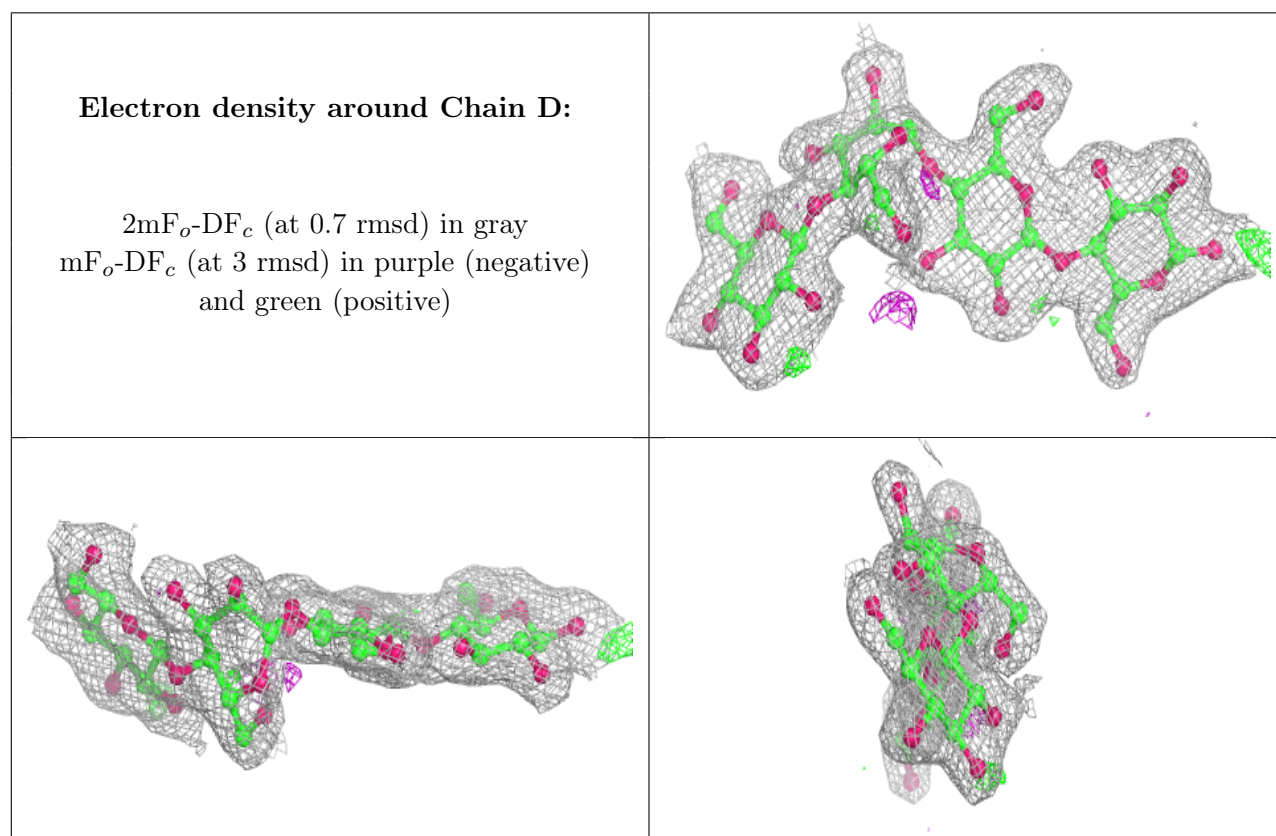
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	BGC	F	2	11/12	0.78	0.18	62,69,77,77	0
3	BGC	F	1	12/12	0.79	0.17	55,70,77,79	0
2	BGC	E	3	11/12	0.91	0.12	24,31,34,35	0
2	BGC	D	4	11/12	0.92	0.11	30,33,36,37	0
2	BGC	G	4	11/12	0.92	0.15	38,42,45,46	0
2	BGC	G	1	12/12	0.93	0.14	29,34,42,47	0
2	BGC	E	2	11/12	0.93	0.10	21,28,31,34	0
2	BGC	D	3	11/12	0.93	0.12	27,28,31,34	0
2	BGC	E	4	11/12	0.93	0.10	23,28,33,35	0
2	BGC	G	3	11/12	0.94	0.16	41,44,46,47	0
2	BGC	G	2	11/12	0.94	0.10	28,33,36,37	0

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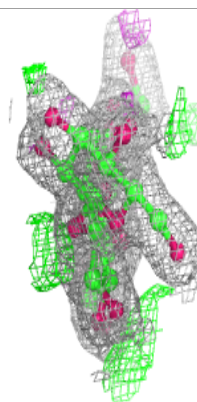
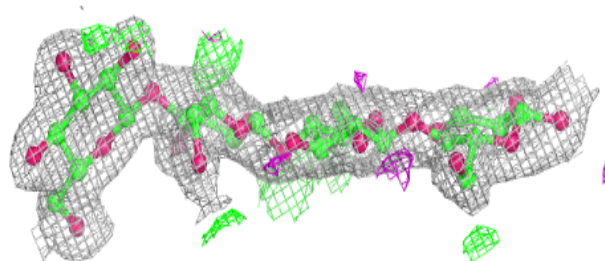
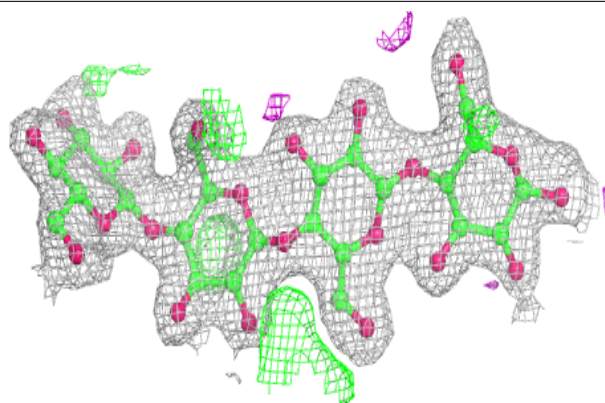
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BGC	E	1	12/12	0.95	0.10	25,32,38,40	0
2	BGC	D	1	12/12	0.95	0.10	22,26,30,37	0
2	BGC	D	2	11/12	0.96	0.09	23,26,30,33	0

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.

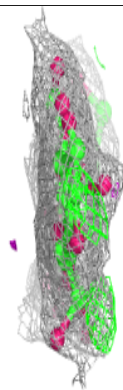
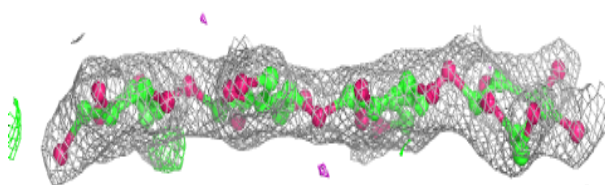
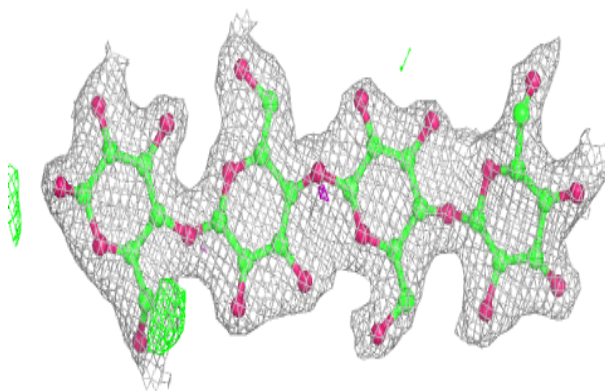


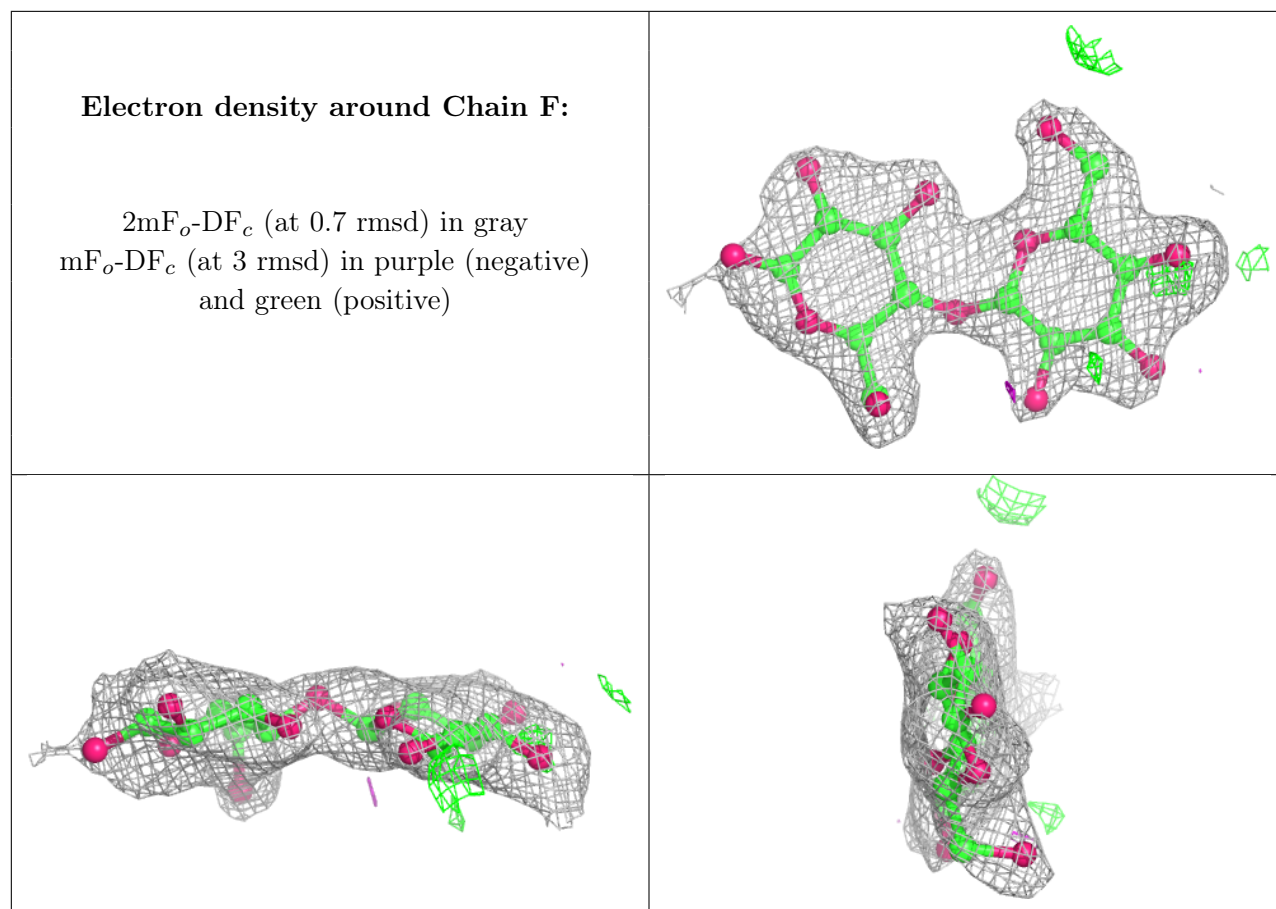
**Electron density around Chain E:**

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

**Electron density around Chain 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 [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.