WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 1, 2023 – 06:58 PM EDT

PDB ID	:	3QHM
Title	:	Crystal analysis of the complex structure, E342A-cellotetraose, of endocellulase from pyrococcus horikoshii
Authors	:	Kim, H.-W.; Ishikawa, K.
Deposited on	:	2011-01-26
Resolution	:	2.01 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

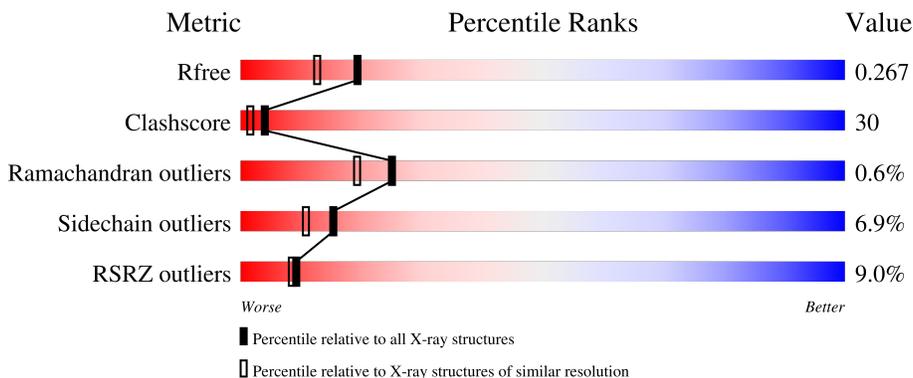|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	Percentile Ranks	Value
Rfree		0.267
Clashscore		30
Ramachandran outliers		0.6%
Sidechain outliers		6.9%
RSRZ outliers		9.0%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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 >=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 <=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	8% — 40% / 34% / 6% · 18%
1	B	458	2% — 68% / 13% · 18%
1	C	458	12% — 48% / 32% · 18%
2	D	4	50% / 50%
2	E	4	100%

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Mol	Chain	Length	Quality of chain
2	G	4	75% 25%
3	F	2	50% 50%

2　Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 9565 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
1	A	377	Total 3067	C 2000	N 502	O 555	S 10	0	0	0
1	B	377	Total 3067	C 2000	N 502	O 555	S 10	0	0	0
1	C	377	Total 3067	C 2000	N 502	O 555	S 10	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	342	ALA	GLU	engineered mutation	UNP O58925
B	342	ALA	GLU	engineered mutation	UNP O58925
C	342	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
2	D	4	Total 45	C 24	O 21	0	0	0
2	E	4	Total 45	C 24	O 21	0	0	0
2	G	4	Total 45	C 24	O 21	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.
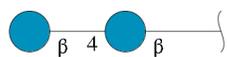
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	F	2	Total 23	C 12	O 11	0	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	67	Total 67	O 67	0	0
4	B	97	Total 97	O 97	0	0
4	C	42	Total 42	O 42	0	0

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.

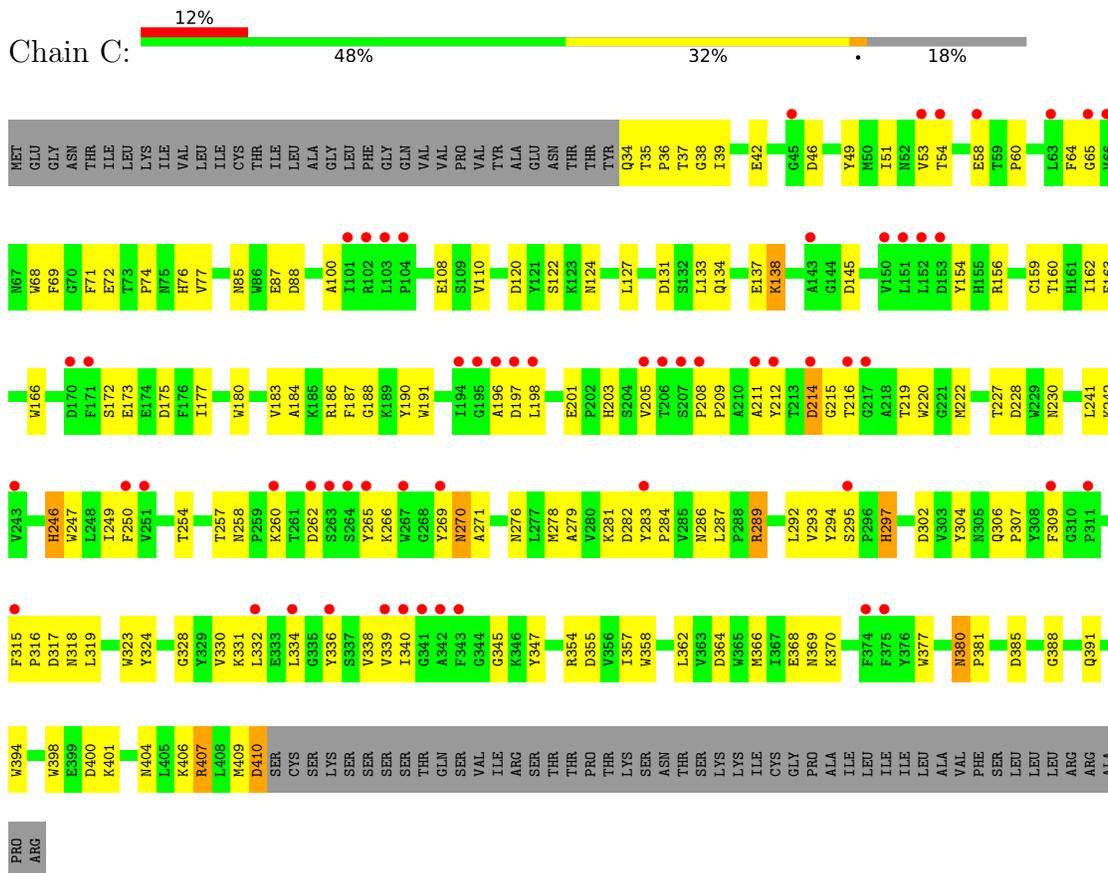- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase
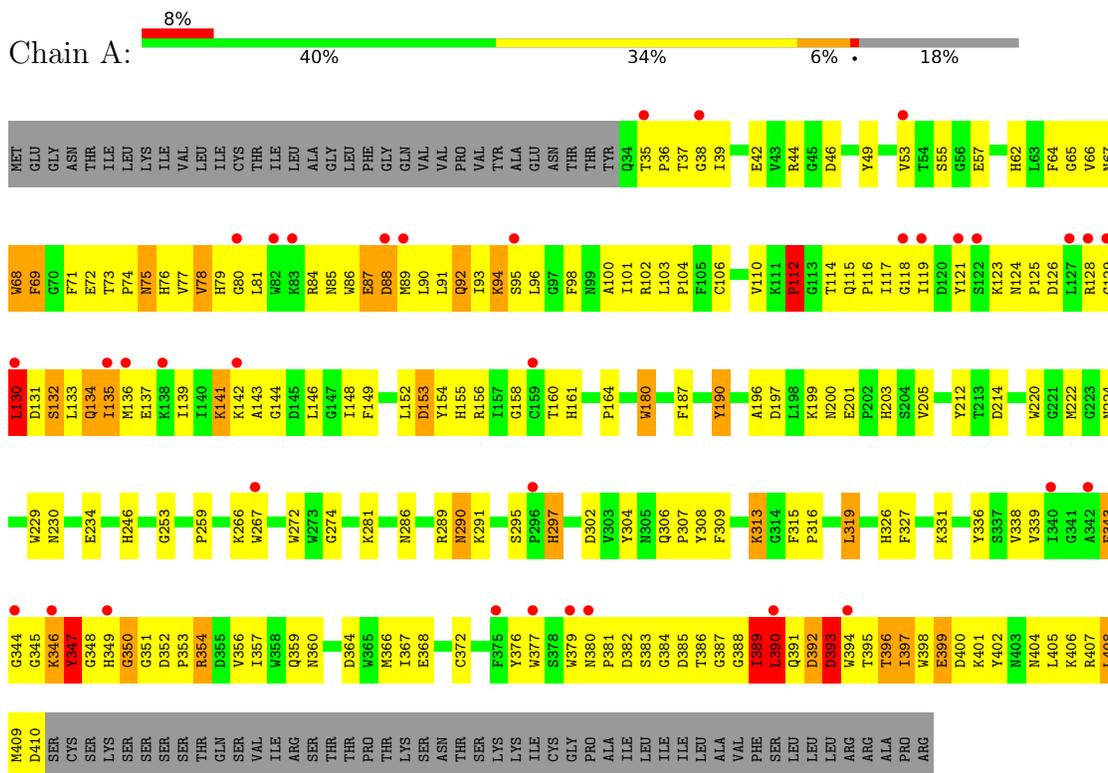
- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase
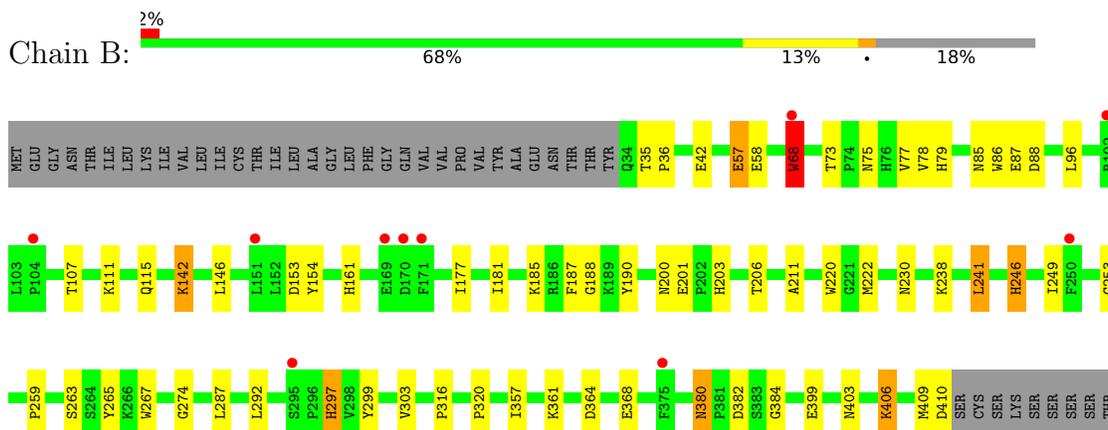
GLN SER VAL ILE ARG SER THR THR PRO THR LYS SER ASN THR SER LYS LYS ILE CYS GLY PRO ALA ILE LEU ILE LEU LEU ALA VAL PHE SER LEU LEU LEU LEU ARG ARG ALA PRO ARG

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

Chain C:

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

Chain D:

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

Chain E:

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

Chain G:

BGC1 BGC2 BGC3 BGC4

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

Chain F:

50%   50%

BGC1 BGC2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.53Å 58.60Å 139.06Å 90.00° 109.69° 90.00°	Depositor
Resolution (Å)	35.25 – 2.01 35.25 – 2.01	Depositor EDS
% Data completeness (in resolution range)	87.7 (35.25-2.01) 87.5 (35.25-2.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 2.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.228 , 0.261 0.236 , 0.267	Depositor DCC
R_{free} test set	3729 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 63.5	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9565	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.39	0/3178	0.81	9/4339 (0.2%)
1	B	0.38	0/3178	0.69	1/4339 (0.0%)
1	C	0.32	0/3178	0.65	0/4339
All	All	0.37	0/9534	0.72	10/13017 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	347	TYR	N-CA-C	-8.56	87.89	111.00
1	A	393	ASP	N-CA-C	-8.50	88.06	111.00
1	A	130	LEU	CA-CB-CG	7.18	131.81	115.30
1	A	348	GLY	N-CA-C	6.17	128.53	113.10
1	A	130	LEU	N-CA-C	6.05	127.34	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	347	TYR	Sidechain

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	3067	0	2909	330	1
1	B	3067	0	2909	67	0
1	C	3067	0	2909	157	0
2	D	45	0	38	3	0
2	E	45	0	39	0	0
2	G	45	0	39	2	0
3	F	23	0	21	2	0
4	A	67	0	0	18	0
4	B	97	0	0	10	2
4	C	42	0	0	5	2
All	All	9565	0	8864	551	3

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 30.

The worst 5 of 551 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:381:PRO:HA	1:A:388:GLY:H	1.10	1.12
1:A:389:ILE:HD13	1:A:401:LYS:HE3	1.31	1.10
1:A:76:HIS:CD2	1:A:114:THR:HG21	1.90	1.05
1:A:402:TYR:HA	4:A:515:HOH:O	1.58	1.02
1:A:131:ASP:O	1:A:133:LEU:N	1.93	1.01

All (3) 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)
4:B:554:HOH:O	4:C:500:HOH:O[4_545]	2.03	0.17
4:B:553:HOH:O	4:C:553:HOH:O[4_545]	2.10	0.10
1:A:95:SER:OG	1:A:354:ARG:NH1[4_556]	2.16	0.04

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	375/458 (82%)	338 (90%)	31 (8%)	6 (2%)	9	4
1	B	375/458 (82%)	361 (96%)	14 (4%)	0	100	100
1	C	375/458 (82%)	354 (94%)	20 (5%)	1 (0%)	41	37
All	All	1125/1374 (82%)	1053 (94%)	65 (6%)	7 (1%)	25	19

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	SER
1	A	384	GLY
1	A	390	LEU
1	A	112	PRO
1	C	215	GLY

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	323/395 (82%)	285 (88%)	38 (12%)	5	3
1	B	323/395 (82%)	311 (96%)	12 (4%)	34	32
1	C	323/395 (82%)	306 (95%)	17 (5%)	22	18
All	All	969/1185 (82%)	902 (93%)	67 (7%)	15	11

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	270	ASN
1	C	287	LEU
1	C	407	ARG
1	A	319	LEU
1	A	313	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	391	GLN
1	C	255	GLN
1	C	62	HIS
1	C	85	ASN
1	C	297	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 ⓘ

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	1.23	2 (16%)	17,17,17	1.58	4 (23%)
2	BGC	D	2	2	11,11,12	0.79	0	15,15,17	1.15	2 (13%)
2	BGC	D	3	2	11,11,12	0.90	0	15,15,17	1.49	2 (13%)
2	BGC	D	4	2	11,11,12	0.68	0	15,15,17	1.27	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	BGC	E	1	2	12,12,12	1.25	0	17,17,17	1.75	3 (17%)
2	BGC	E	2	2	11,11,12	0.89	0	15,15,17	1.14	2 (13%)
2	BGC	E	3	2	11,11,12	1.03	1 (9%)	15,15,17	1.20	1 (6%)
2	BGC	E	4	2	11,11,12	0.73	0	15,15,17	0.96	1 (6%)
3	BGC	F	1	3	12,12,12	0.51	0	17,17,17	0.93	2 (11%)
3	BGC	F	2	3	11,11,12	0.32	0	15,15,17	0.99	1 (6%)
2	BGC	G	1	2	12,12,12	1.39	0	17,17,17	2.15	5 (29%)
2	BGC	G	2	2	11,11,12	0.88	0	15,15,17	1.08	1 (6%)
2	BGC	G	3	2	11,11,12	0.89	1 (9%)	15,15,17	1.24	2 (13%)
2	BGC	G	4	2	11,11,12	0.81	0	15,15,17	1.06	1 (6%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	BGC	C4-C5	2.15	1.57	1.53
2	G	3	BGC	O5-C1	2.15	1.47	1.43
2	D	1	BGC	O5-C5	2.09	1.49	1.44
2	D	1	BGC	O4-C4	2.03	1.47	1.43

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1	BGC	C1-C2-C3	-4.79	100.37	110.31
2	G	1	BGC	C1-O5-C5	-4.38	105.40	113.66
2	D	3	BGC	C1-C2-C3	-4.03	104.72	109.67
2	E	1	BGC	C1-O5-C5	-3.85	106.39	113.66
2	E	1	BGC	C1-C2-C3	-3.80	102.44	110.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

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

Oligosaccharide Chain D

Bond lengths   Bond angles

Torsions   Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F
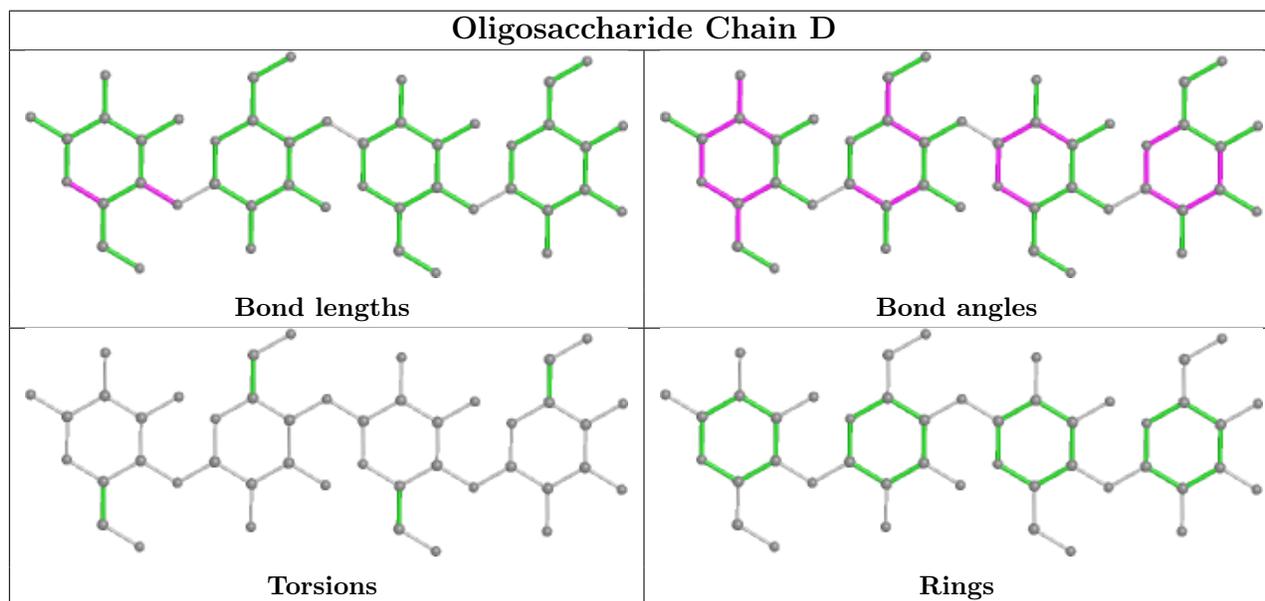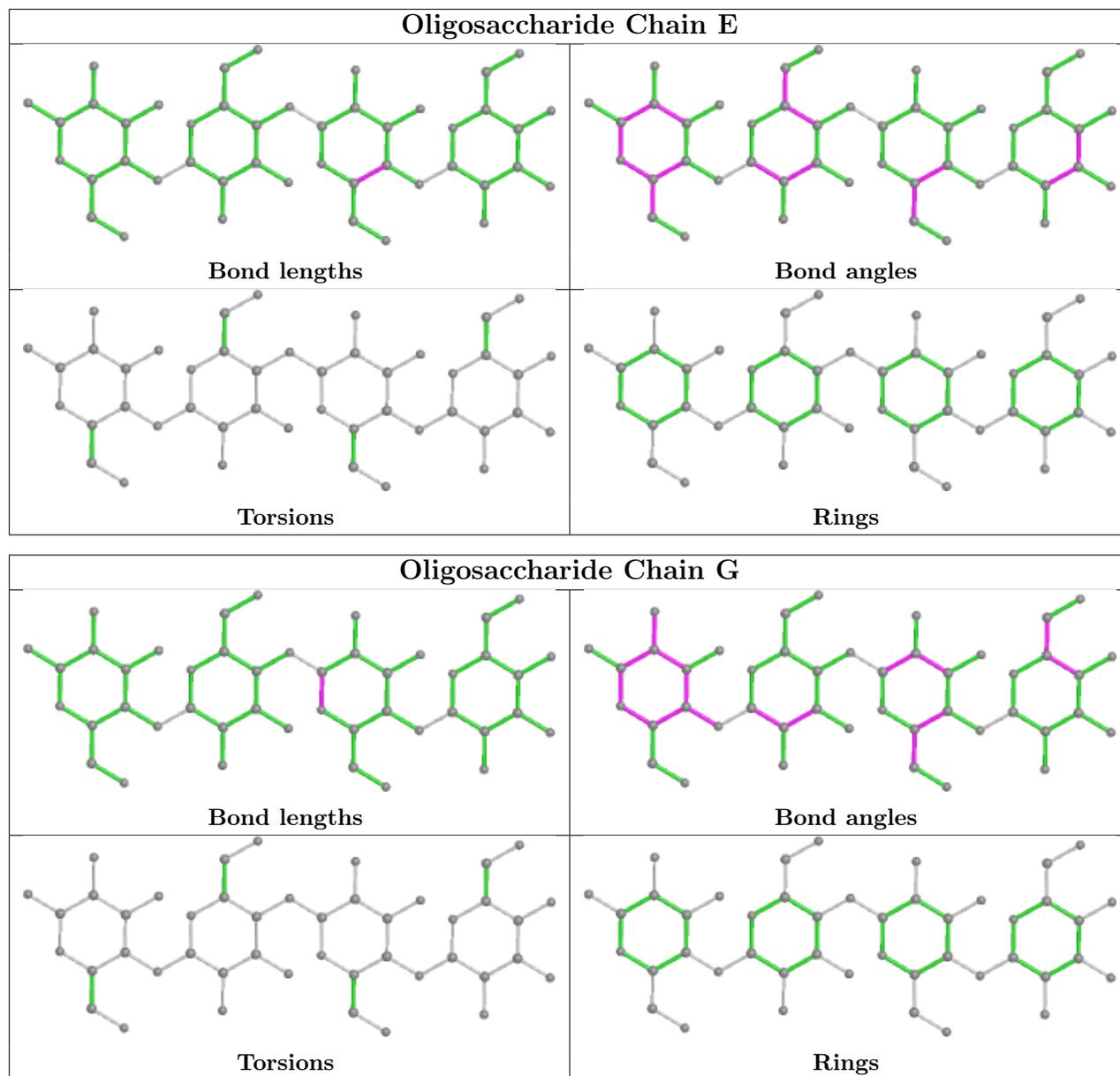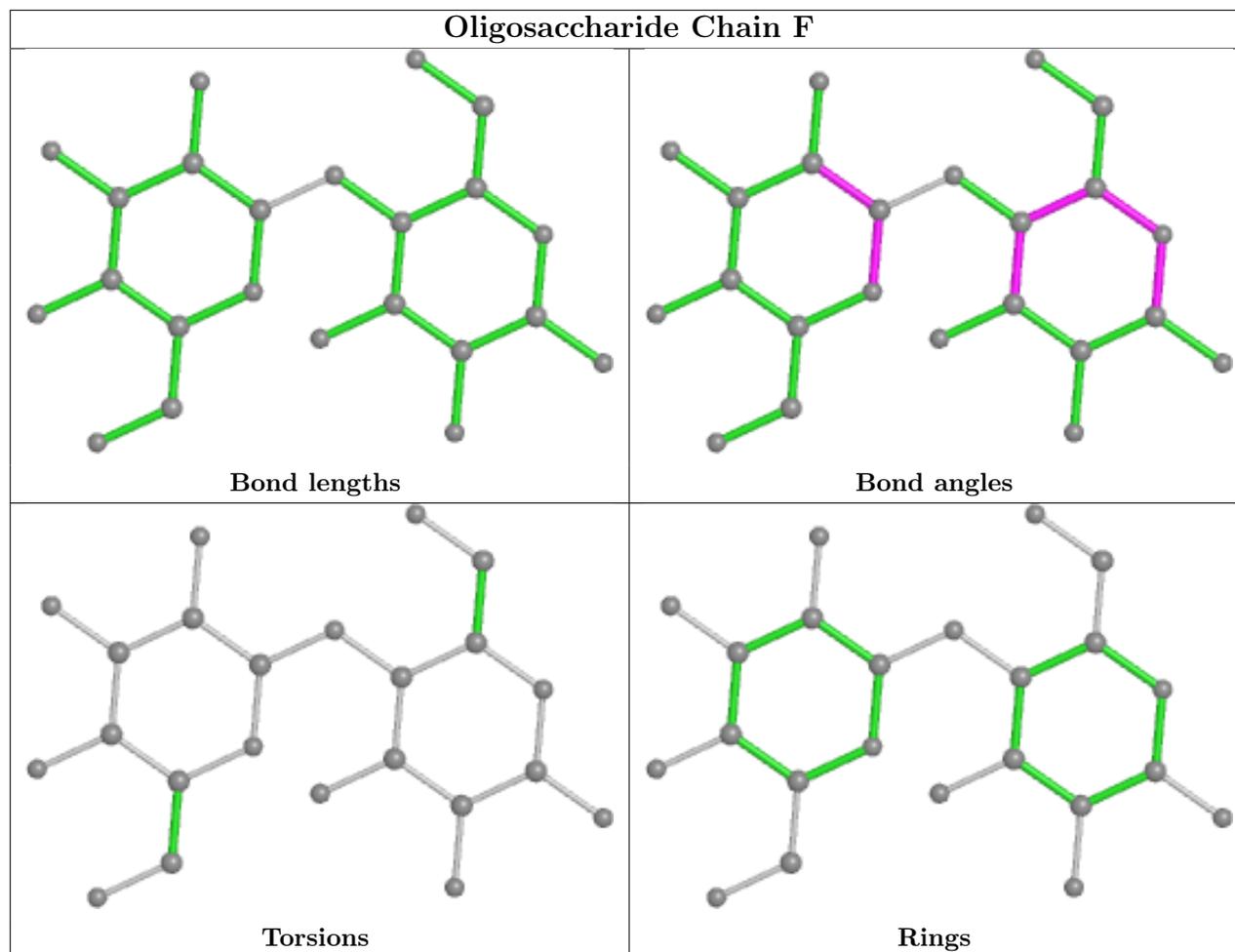
5.6 Ligand geometry (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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^2)	Q<0.9
1	A	377/458 (82%)	0.54	35 (9%)	8	8	26, 52, 84, 113	2 (0%)
1	B	377/458 (82%)	-0.11	10 (2%)	54	53	20, 33, 55, 85	3 (0%)
1	C	377/458 (82%)	0.62	57 (15%)	2	1	29, 56, 81, 101	2 (0%)
All	All	1131/1374 (82%)	0.35	102 (9%)	9	8	20, 46, 79, 113	7 (0%)

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	LEU	6.8
1	C	269	TYR	5.6
1	A	122	SER	5.5
1	C	151	LEU	5.4
1	C	342	ALA	4.8

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, 95th 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.
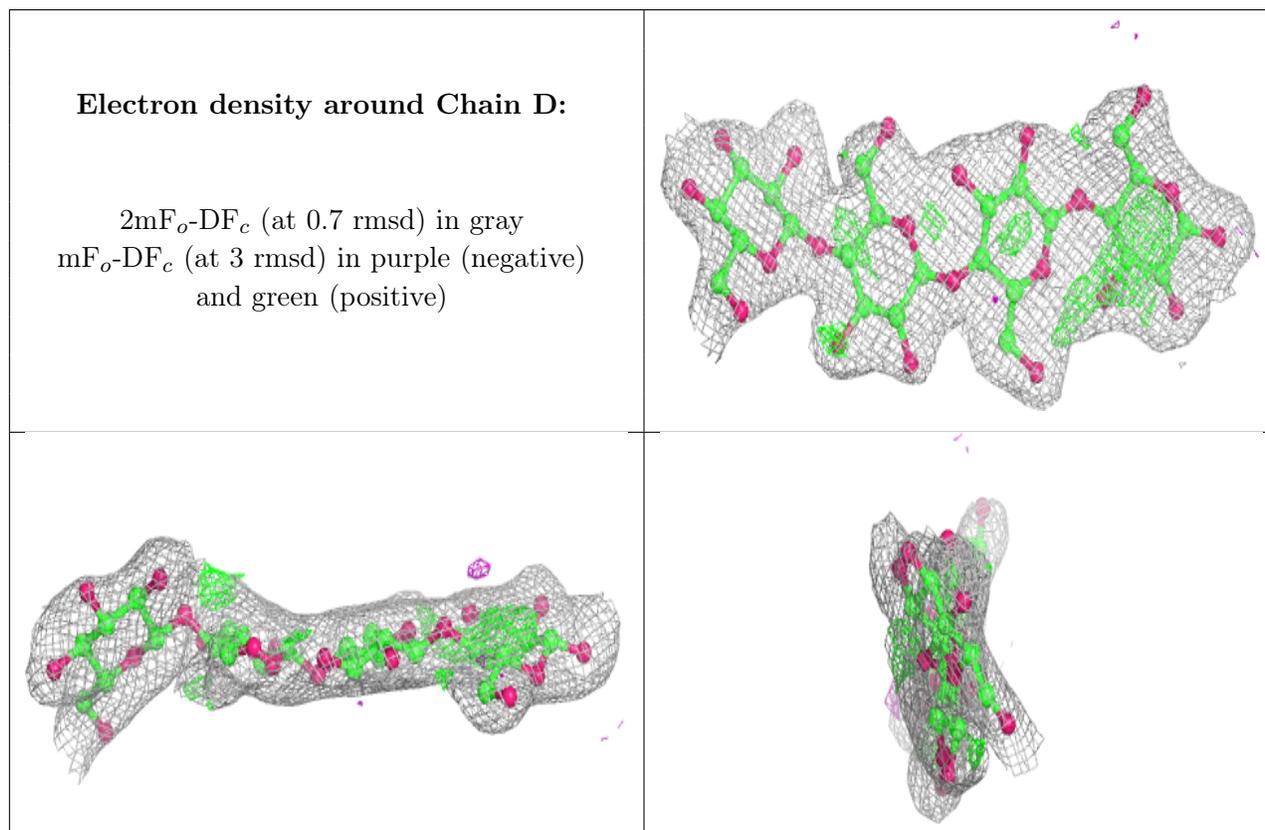
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	G	1	12/12	0.85	0.17	50,57,67,68	0
3	BGC	F	2	11/12	0.85	0.13	63,68,75,77	0
2	BGC	G	4	11/12	0.87	0.17	49,58,69,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	D	3	11/12	0.88	0.14	56,61,65,71	0
3	BGC	F	1	12/12	0.89	0.11	58,68,75,78	0
2	BGC	E	1	12/12	0.89	0.14	36,42,49,66	0
2	BGC	D	1	12/12	0.90	0.14	38,48,59,71	0
2	BGC	D	2	11/12	0.90	0.14	39,44,60,64	0
2	BGC	D	4	11/12	0.91	0.16	46,56,70,72	0
2	BGC	E	2	11/12	0.92	0.11	28,35,42,47	0
2	BGC	G	2	11/12	0.93	0.10	40,46,51,52	0
2	BGC	G	3	11/12	0.94	0.15	53,61,67,68	0
2	BGC	E	4	11/12	0.94	0.18	31,33,41,43	0
2	BGC	E	3	11/12	0.95	0.15	23,26,37,55	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 D:

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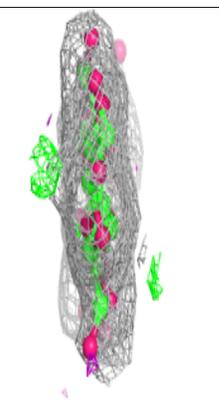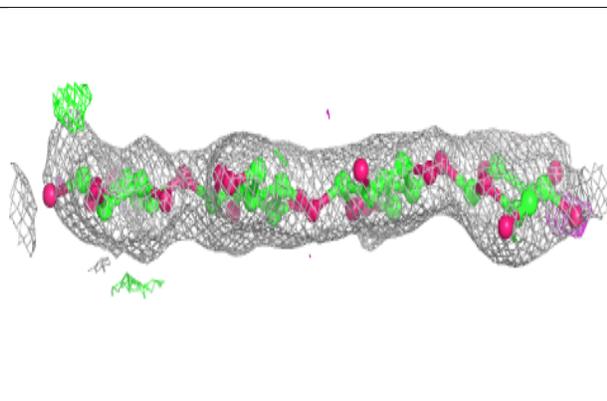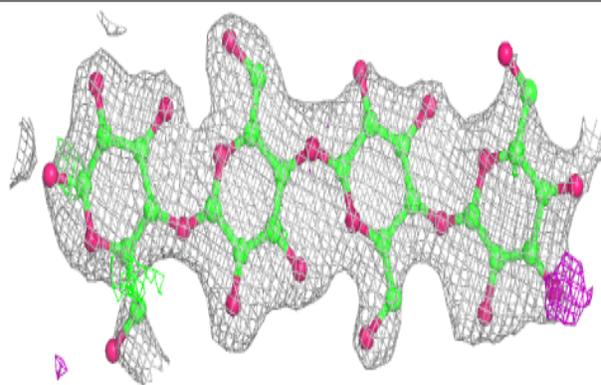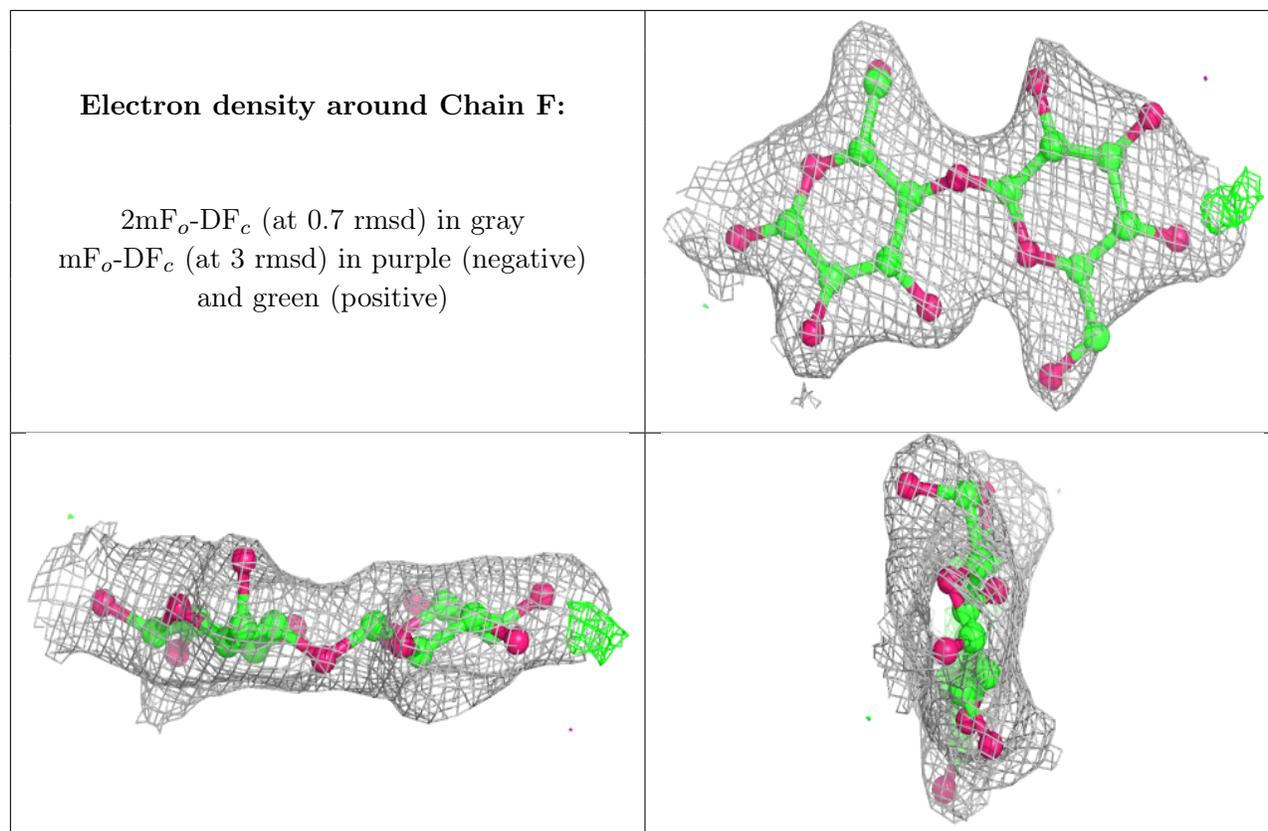and green (positive)

Electron density around Chain E:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
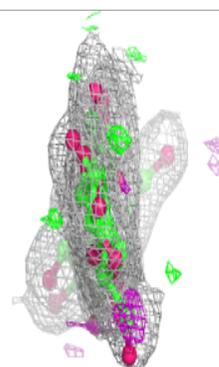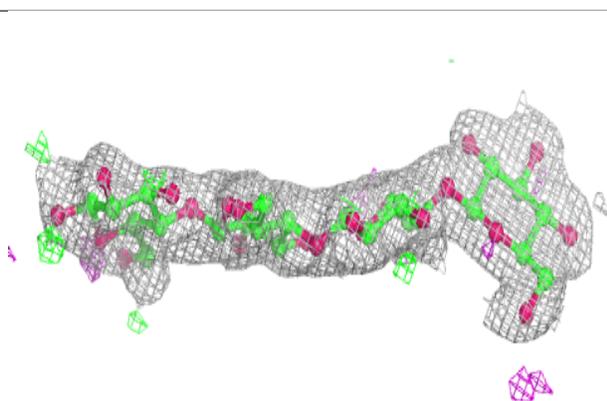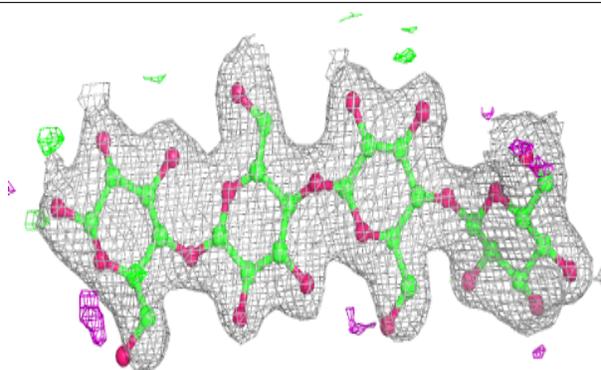
Electron density around Chain G:

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

Electron density around Chain F:

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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.