



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2023 – 09:32 PM EDT

PDB ID : 3A8E  
Title : The structure of AxcesD octamer complexed with cellopentaose  
Authors : Hu, S.Q.; Tajima, K.; Zhou, Y.; Yao, M.; Tanaka, I.  
Deposited on : 2009-10-05  
Resolution : 3.00 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

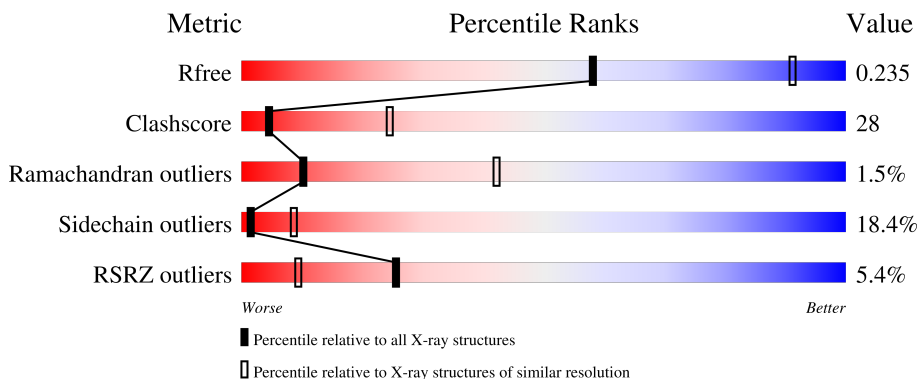
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	162	 6% 55% 30% 7% 9%
1	B	162	 5% 61% 30% 6% ..
1	C	162	 4% 54% 32% 12% .
1	D	162	 6% 51% 31% 10% 9%
2	E	5	 20% 80%

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BGC	E	1	-	-	-	X
2	BGC	E	3	-	-	-	X
2	BGC	E	4	-	-	-	X
2	BGC	E	5	-	-	-	X
2	BGC	F	1[A]	-	-	-	X
2	BGC	F	1[B]	-	-	-	X
2	BGC	F	2[A]	-	-	-	X
2	BGC	F	2[B]	-	-	-	X
2	BGC	F	3[A]	-	-	-	X
2	BGC	F	3[B]	-	-	-	X
2	BGC	F	4[A]	-	-	X	X
2	BGC	F	4[B]	-	-	X	X
2	BGC	F	5[A]	-	-	-	X
2	BGC	F	5[B]	-	-	-	X
2	BGC	G	1	-	-	-	X
2	BGC	G	2	-	-	-	X
2	BGC	G	3	-	-	-	X
2	BGC	G	4	-	-	X	X

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 5230 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 Cellulose synthase operon protein D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	148	1162	740	196	221	5	0	0	0
1	B	158	1247	789	219	234	5	0	0	0
1	C	159	1257	795	222	235	5	0	0	0
1	D	148	1162	740	196	221	5	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

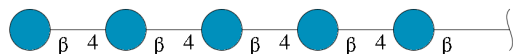
Chain	Residue	Modelled	Actual	Comment	Reference
A	157	HIS	-	expression tag	UNP P37719
A	158	HIS	-	expression tag	UNP P37719
A	159	HIS	-	expression tag	UNP P37719
A	160	HIS	-	expression tag	UNP P37719
A	161	HIS	-	expression tag	UNP P37719
A	162	HIS	-	expression tag	UNP P37719
B	157	HIS	-	expression tag	UNP P37719
B	158	HIS	-	expression tag	UNP P37719
B	159	HIS	-	expression tag	UNP P37719
B	160	HIS	-	expression tag	UNP P37719
B	161	HIS	-	expression tag	UNP P37719
B	162	HIS	-	expression tag	UNP P37719
C	157	HIS	-	expression tag	UNP P37719
C	158	HIS	-	expression tag	UNP P37719
C	159	HIS	-	expression tag	UNP P37719
C	160	HIS	-	expression tag	UNP P37719
C	161	HIS	-	expression tag	UNP P37719
C	162	HIS	-	expression tag	UNP P37719
D	157	HIS	-	expression tag	UNP P37719
D	158	HIS	-	expression tag	UNP P37719
D	159	HIS	-	expression tag	UNP P37719

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Chain	Residue	Modelled	Actual	Comment	Reference
D	160	HIS	-	expression tag	UNP P37719
D	161	HIS	-	expression tag	UNP P37719
D	162	HIS	-	expression tag	UNP P37719

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-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	E	5	Total	C	O	0	0	0
			56	30	26			
2	F	5	Total	C	O	0	5	0
			112	60	52			
2	G	5	Total	C	O	0	0	0
			56	30	26			

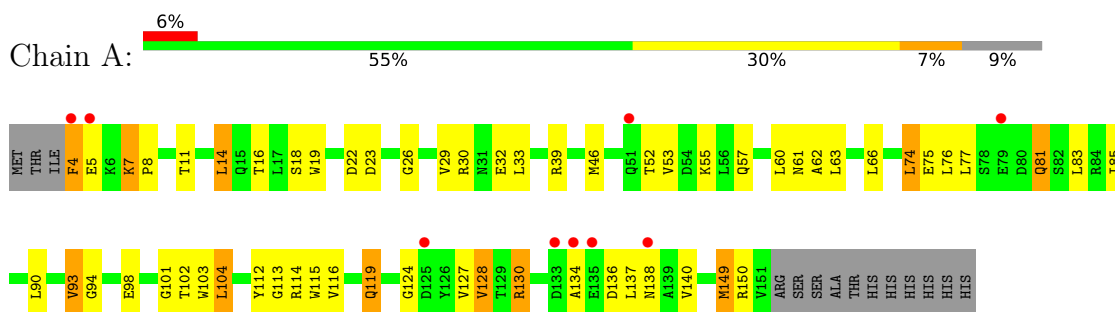
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total	O	0	0
			45	45		
3	B	42	Total	O	0	0
			42	42		
3	C	46	Total	O	0	0
			46	46		
3	D	45	Total	O	0	0
			45	45		

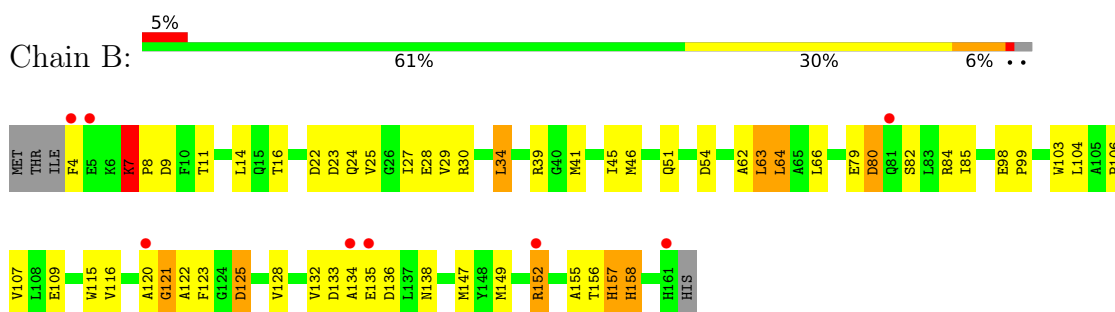
### 3 Residue-property plots [i](#)

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

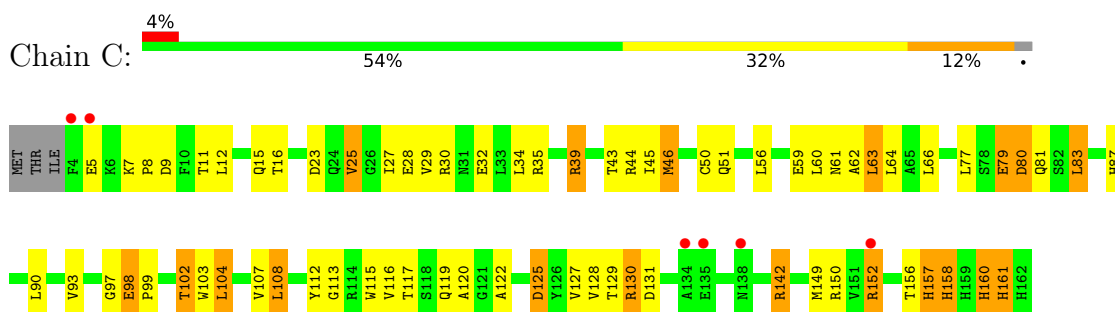
- Molecule 1: Cellulose synthase operon protein D



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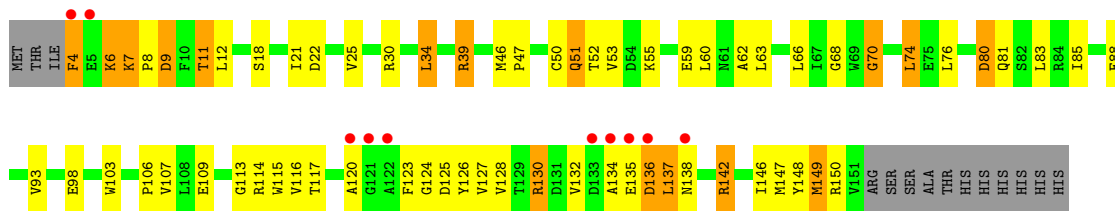


- Molecule 1: Cellulose synthase operon protein D



- Molecule 1: Cellulose synthase operon protein D





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



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.88Å 132.88Å 216.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 3.00 19.94 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.94-3.00) 100.0 (19.94-3.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.78 (at 2.98Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.242 , 0.293 0.236 , 0.235	Depositor DCC
$R_{free}$ test set	2015 reflections (10.24%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.8	Xtrriage
Anisotropy	0.190	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 55.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.39$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5230	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.53 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.4891e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.38	0/1185	0.63	1/1614 (0.1%)
1	B	0.40	0/1275	0.63	0/1736
1	C	0.38	0/1286	0.63	0/1751
1	D	0.40	0/1185	0.67	0/1614
All	All	0.39	0/4931	0.64	1/6715 (0.0%)

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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	66	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	7	LYS	Peptide

## 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	1162	0	1160	48	0
1	B	1247	0	1230	73	0
1	C	1257	0	1237	76	0
1	D	1162	0	1160	64	0
2	E	56	0	48	10	0
2	F	112	0	96	34	0
2	G	56	0	48	14	0
3	A	45	0	0	3	0
3	B	42	0	0	1	0
3	C	46	0	0	3	0
3	D	45	0	0	3	0
All	All	5230	0	4979	285	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 28.

All (285) 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:D:7:LYS:HB3	1:D:8:PRO:CD	1.69	1.22
1:A:7:LYS:HB3	1:A:8:PRO:CD	1.69	1.21
1:B:155:ALA:HB1	1:B:158:HIS:CG	1.82	1.13
1:A:7:LYS:HB3	1:A:8:PRO:HD2	1.31	1.09
1:B:7:LYS:HB3	1:B:8:PRO:CD	1.84	1.07
1:B:7:LYS:HB3	1:B:8:PRO:HD3	1.36	1.06
1:D:7:LYS:HB3	1:D:8:PRO:HD3	1.37	1.03
1:A:112:TYR:HA	3:A:214:HOH:O	1.58	1.03
1:B:156:THR:N	1:B:158:HIS:CD2	2.32	0.97
1:B:158:HIS:CD2	1:B:158:HIS:H	1.63	0.96
2:F:3[A]:BGC:H3	2:F:4[A]:BGC:C2	1.95	0.96
2:F:3[B]:BGC:H3	2:F:4[B]:BGC:C2	1.97	0.95
1:B:66:LEU:HD12	2:F:4[B]:BGC:H3	1.50	0.94
1:D:39:ARG:HG2	1:D:39:ARG:HH11	1.27	0.93
2:E:3:BGC:H3	2:E:4:BGC:C2	1.99	0.92
2:G:3:BGC:H3	2:G:4:BGC:C2	2.00	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:LEU:HD12	2:F:4[A]:BGC:H3	1.52	0.91
1:C:7:LYS:HE2	1:C:7:LYS:HA	1.48	0.91
2:F:3[A]:BGC:H3	2:F:4[A]:BGC:H2	1.53	0.91
1:A:30:ARG:HD2	1:A:103:TRP:NE1	1.86	0.90
1:A:81:GLN:HA	1:A:81:GLN:HE21	1.33	0.90
1:C:128:VAL:HG22	1:C:149:MET:SD	2.12	0.90
1:D:30:ARG:HD2	1:D:103:TRP:HE1	1.35	0.89
1:D:62:ALA:HA	2:G:1:BGC:O3	1.72	0.89
1:B:80:ASP:HB2	1:B:82:SER:HB3	1.55	0.87
1:B:155:ALA:HB1	1:B:158:HIS:CB	2.05	0.86
2:G:3:BGC:H3	2:G:4:BGC:H2	1.58	0.85
1:B:156:THR:HG23	1:B:157:HIS:HD2	1.38	0.85
1:D:7:LYS:HB3	1:D:8:PRO:HD2	1.56	0.85
2:F:3[B]:BGC:H3	2:F:4[B]:BGC:H2	1.57	0.85
1:A:7:LYS:HB3	1:A:8:PRO:HD3	1.58	0.84
1:C:64:LEU:HD12	3:C:270:HOH:O	1.78	0.84
1:C:156:THR:HB	1:C:158:HIS:CD2	2.13	0.84
2:E:3:BGC:H3	2:E:4:BGC:H2	1.59	0.84
1:D:9:ASP:OD1	2:F:4[B]:BGC:H4	1.77	0.83
1:A:62:ALA:HB1	2:E:5:BGC:O3	1.77	0.83
1:D:30:ARG:HD2	1:D:103:TRP:NE1	1.91	0.83
1:D:7:LYS:CB	1:D:8:PRO:CD	2.54	0.82
1:C:9:ASP:OD2	2:G:4:BGC:H4	1.81	0.81
1:A:11:THR:HG21	2:F:5[A]:BGC:H4	1.61	0.80
1:C:7:LYS:HB3	1:C:8:PRO:CD	2.12	0.79
1:B:134:ALA:O	1:B:135:GLU:HG2	1.82	0.79
1:C:50:CYS:H	1:C:119:GLN:NE2	1.81	0.79
1:A:7:LYS:CB	1:A:8:PRO:CD	2.57	0.78
1:A:81:GLN:HE21	1:A:81:GLN:CA	1.95	0.77
1:B:158:HIS:H	1:B:158:HIS:HD2	1.32	0.77
1:B:155:ALA:HB1	1:B:158:HIS:HB2	1.66	0.77
1:B:158:HIS:CD2	1:B:158:HIS:N	2.47	0.77
1:A:81:GLN:HA	1:A:81:GLN:NE2	1.96	0.77
1:C:7:LYS:HB3	1:C:8:PRO:HD2	1.66	0.76
1:C:62:ALA:HB1	2:F:5[A]:BGC:O3	1.86	0.76
1:C:62:ALA:HA	2:F:1[B]:BGC:O3	1.86	0.76
1:D:132:VAL:HG21	1:D:137:LEU:HA	1.68	0.76
1:B:62:ALA:HB1	2:F:5[B]:BGC:O3	1.87	0.75
1:B:66:LEU:HD12	2:F:2[A]:BGC:H2	1.69	0.74
1:C:160:HIS:O	1:C:160:HIS:ND1	2.19	0.74
1:C:50:CYS:H	1:C:119:GLN:HE22	1.34	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ASP:OD1	1:A:30:ARG:HD3	1.88	0.73
1:A:115:TRP:CE3	3:A:214:HOH:O	2.42	0.73
2:G:1:BGC:H6C1	2:G:2:BGC:C1	2.18	0.73
2:E:1:BGC:H6C1	2:E:2:BGC:C1	2.18	0.72
1:B:85:ILE:HD11	1:B:149:MET:HE3	1.69	0.72
1:A:4:PHE:O	1:A:5:GLU:HG2	1.89	0.72
1:B:156:THR:HG23	1:B:157:HIS:CD2	2.25	0.71
1:C:7:LYS:HA	1:C:7:LYS:CE	2.19	0.71
1:D:9:ASP:OD1	2:F:2[A]:BGC:H3	1.90	0.70
1:C:30:ARG:HD2	1:C:103:TRP:NE1	2.06	0.70
2:F:1[B]:BGC:H6C1	2:F:2[B]:BGC:C1	2.21	0.70
1:D:74:LEU:HD12	1:D:85:ILE:HG12	1.74	0.70
1:B:41:MET:HE1	1:B:107:VAL:HG11	1.74	0.70
2:F:1[A]:BGC:H6C1	2:F:2[A]:BGC:C1	2.22	0.70
1:B:30:ARG:HD2	1:B:103:TRP:NE1	2.07	0.69
1:A:93:VAL:HG13	1:A:93:VAL:O	1.93	0.69
1:D:51:GLN:HG2	1:D:55:LYS:HD3	1.74	0.69
1:C:127:VAL:HG13	1:C:152:ARG:HG2	1.74	0.68
1:A:7:LYS:CB	1:A:8:PRO:HD2	2.17	0.68
1:B:62:ALA:HA	2:F:1[A]:BGC:O3	1.94	0.68
1:C:152:ARG:HH21	1:C:152:ARG:HG3	1.59	0.68
1:D:137:LEU:HD12	1:D:137:LEU:H	1.59	0.67
1:B:128:VAL:HG22	1:B:149:MET:SD	2.35	0.67
1:A:62:ALA:HA	2:E:5:BGC:O4	1.94	0.67
1:C:97:GLY:C	1:C:98:GLU:OE2	2.33	0.67
1:B:7:LYS:CB	1:B:8:PRO:CD	2.68	0.66
1:B:157:HIS:CD2	1:B:157:HIS:H	2.10	0.66
1:A:14:LEU:HB3	1:A:93:VAL:CG2	2.25	0.66
1:D:125:ASP:O	1:D:126:TYR:HD1	1.78	0.66
1:A:62:ALA:O	2:E:5:BGC:H3	1.96	0.66
1:D:4:PHE:N	1:D:4:PHE:CD1	2.63	0.65
1:D:130:ARG:HA	1:D:147:MET:HG2	1.76	0.65
1:A:14:LEU:HB3	1:A:93:VAL:HG21	1.79	0.65
1:B:41:MET:CE	1:B:107:VAL:CG1	2.74	0.65
1:A:30:ARG:NH2	1:A:98:GLU:OE2	2.25	0.64
1:D:39:ARG:HG2	1:D:39:ARG:NH1	2.05	0.64
2:E:3:BGC:H3	2:E:4:BGC:O2	1.97	0.64
2:F:3[B]:BGC:H3	2:F:4[B]:BGC:O2	1.97	0.64
1:D:7:LYS:CB	1:D:8:PRO:HD2	2.25	0.64
1:D:109:GLU:CD	1:D:130:ARG:HB3	2.18	0.64
1:B:157:HIS:N	1:B:158:HIS:CD2	2.66	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:HIS:N	1:B:158:HIS:HD2	1.96	0.64
1:C:116:VAL:HG21	1:C:149:MET:SD	2.39	0.63
1:C:152:ARG:HH21	1:C:152:ARG:CG	2.11	0.63
2:F:3[A]:BGC:H3	2:F:4[A]:BGC:O2	1.98	0.63
1:C:98:GLU:OE2	1:C:98:GLU:N	2.33	0.62
1:D:132:VAL:HG11	1:D:136:ASP:O	2.00	0.62
1:A:30:ARG:HD2	1:A:103:TRP:HE1	1.65	0.61
1:C:25:VAL:HG13	1:C:29:VAL:HB	1.82	0.61
1:D:34:LEU:HB3	1:D:106:PRO:HB2	1.82	0.61
1:B:135:GLU:HA	1:B:138:ASN:HB2	1.82	0.61
1:C:7:LYS:HE2	1:C:7:LYS:CA	2.26	0.61
1:D:117:THR:HG23	1:D:124:GLY:HA2	1.83	0.60
1:D:22:ASP:OD1	1:D:30:ARG:HD2	2.02	0.60
2:G:3:BGC:H3	2:G:4:BGC:O2	2.01	0.60
1:D:107:VAL:HG23	3:D:200:HOH:O	2.01	0.60
1:B:155:ALA:C	1:B:158:HIS:CD2	2.75	0.59
1:B:157:HIS:HD2	1:B:157:HIS:H	1.50	0.59
1:C:113:GLY:HA2	1:C:149:MET:HE1	1.84	0.59
1:C:127:VAL:CG1	1:C:152:ARG:HG2	2.32	0.59
1:D:11:THR:HG21	2:F:5[B]:BGC:O5	2.03	0.59
1:B:41:MET:HE3	1:B:107:VAL:CG1	2.33	0.58
1:C:9:ASP:CG	2:G:4:BGC:H4	2.22	0.58
1:C:99:PRO:O	1:C:102:THR:HB	2.04	0.58
1:B:7:LYS:HB3	1:B:8:PRO:HD2	1.84	0.58
1:D:22:ASP:OD1	1:D:30:ARG:CD	2.52	0.58
1:D:113:GLY:HA2	1:D:149:MET:HE1	1.86	0.57
1:B:120:ALA:O	1:B:121:GLY:O	2.22	0.57
1:C:152:ARG:HG3	1:C:152:ARG:NH2	2.20	0.57
1:B:41:MET:HE1	1:B:107:VAL:CG1	2.34	0.57
1:D:9:ASP:OD2	1:D:9:ASP:C	2.42	0.57
1:C:156:THR:CB	1:C:158:HIS:CD2	2.87	0.56
1:B:156:THR:N	1:B:158:HIS:HD2	2.01	0.56
2:F:3[A]:BGC:C3	2:F:4[A]:BGC:H2	2.31	0.56
1:A:62:ALA:HB1	2:E:5:BGC:HC	1.71	0.56
1:D:132:VAL:CG1	1:D:134:ALA:HB3	2.36	0.56
1:C:11:THR:HG21	2:G:5:BGC:H4	1.87	0.55
1:B:123:PHE:HD1	1:B:123:PHE:N	2.04	0.55
1:C:39:ARG:O	1:C:43:THR:HG23	2.06	0.55
1:D:70:GLY:HA3	1:D:88:GLU:O	2.05	0.55
1:B:34:LEU:HB3	1:B:106:PRO:HB2	1.89	0.55
1:C:90:LEU:HD11	1:C:104:LEU:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:VAL:O	1:A:93:VAL:CG1	2.54	0.55
1:B:54:ASP:OD1	1:D:142:ARG:NH2	2.39	0.55
1:C:11:THR:HB	2:G:5:BGC:H2	1.89	0.55
1:D:132:VAL:O	1:D:135:GLU:HA	2.07	0.55
1:B:156:THR:C	1:B:158:HIS:HD2	2.09	0.54
1:D:127:VAL:O	1:D:149:MET:HA	2.07	0.54
1:B:66:LEU:HD13	2:F:5[B]:BGC:O2	2.07	0.54
1:B:123:PHE:N	1:B:123:PHE:CD1	2.74	0.54
2:F:3[B]:BGC:C3	2:F:4[B]:BGC:H2	2.36	0.54
1:B:155:ALA:CB	1:B:158:HIS:HB2	2.35	0.54
1:C:30:ARG:HH22	1:C:98:GLU:CD	2.11	0.54
1:C:66:LEU:HD12	2:F:4[A]:BGC:C3	2.32	0.54
1:B:41:MET:CE	1:B:107:VAL:HG13	2.38	0.53
1:B:125:ASP:OD1	1:B:152:ARG:HD2	2.08	0.53
1:D:60:LEU:HD12	1:D:74:LEU:HD21	1.91	0.53
1:C:50:CYS:N	1:C:119:GLN:NE2	2.56	0.53
1:D:51:GLN:HG2	1:D:55:LYS:CD	2.38	0.53
1:D:11:THR:HG21	2:F:4[B]:BGC:H6C2	1.90	0.53
1:C:112:TYR:O	1:C:116:VAL:HG22	2.09	0.53
1:A:81:GLN:CA	1:A:81:GLN:NE2	2.66	0.52
1:B:156:THR:H	1:B:158:HIS:CD2	2.22	0.52
1:D:135:GLU:O	1:D:135:GLU:HG2	2.09	0.52
1:D:9:ASP:OD1	2:F:4[B]:BGC:C4	2.54	0.52
1:D:21:ILE:O	1:D:25:VAL:HG22	2.10	0.52
1:C:90:LEU:HD13	1:C:108:LEU:HD22	1.92	0.52
1:B:30:ARG:HD2	1:B:103:TRP:HE1	1.74	0.51
1:B:85:ILE:HD11	1:B:149:MET:CE	2.39	0.51
1:D:39:ARG:HH11	1:D:39:ARG:CG	2.11	0.51
1:A:11:THR:HG21	2:F:5[A]:BGC:C4	2.35	0.51
1:C:28:GLU:HA	1:C:28:GLU:OE1	2.10	0.51
2:G:4:BGC:C6	2:G:5:BGC:O5	2.58	0.51
1:B:28:GLU:OE2	1:B:28:GLU:HA	2.11	0.51
1:B:11:THR:HG21	2:E:1:BGC:H3	1.93	0.51
1:A:39:ARG:HD2	1:A:114:ARG:HD3	1.91	0.51
1:C:125:ASP:N	1:C:125:ASP:OD2	2.44	0.51
1:A:90:LEU:HD11	1:A:104:LEU:HB3	1.93	0.50
1:A:116:VAL:O	1:A:119:GLN:HB2	2.11	0.50
1:B:157:HIS:CD2	1:B:157:HIS:N	2.77	0.50
1:D:52:THR:OG1	1:D:55:LYS:HG3	2.12	0.50
1:D:132:VAL:CG2	1:D:137:LEU:HA	2.38	0.50
2:E:3:BGC:C3	2:E:4:BGC:H2	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:HIS:O	1:C:161:HIS:ND1	2.44	0.50
1:D:126:TYR:HA	1:D:150:ARG:O	2.12	0.50
1:A:60:LEU:HD22	1:A:115:TRP:CE3	2.46	0.49
1:C:8:PRO:HB3	1:D:68:GLY:O	2.12	0.49
1:D:132:VAL:HG12	1:D:135:GLU:N	2.28	0.49
1:C:7:LYS:HD3	1:C:8:PRO:HD3	1.93	0.49
1:A:113:GLY:HA2	1:A:149:MET:HE1	1.94	0.48
1:B:155:ALA:CB	1:B:158:HIS:CG	2.75	0.48
1:C:157:HIS:ND1	1:C:157:HIS:N	2.57	0.48
1:A:134:ALA:HA	1:A:137:LEU:HB2	1.95	0.48
1:B:66:LEU:HD12	2:F:4[B]:BGC:C3	2.33	0.48
1:D:132:VAL:HG21	3:D:228:HOH:O	2.13	0.48
1:B:25:VAL:HG13	1:B:29:VAL:HB	1.95	0.48
1:B:85:ILE:CD1	1:B:149:MET:CE	2.91	0.48
1:C:50:CYS:SG	1:C:59:GLU:HG3	2.53	0.48
1:A:94:GLY:O	1:A:101:GLY:HA2	2.14	0.48
1:A:52:THR:OG1	1:A:55:LYS:HG3	2.14	0.47
1:B:41:MET:HE3	1:B:107:VAL:HG13	1.96	0.47
1:B:116:VAL:CG1	1:B:123:PHE:HD2	2.26	0.47
1:D:116:VAL:HG21	1:D:149:MET:HG2	1.97	0.47
1:D:130:ARG:O	1:D:146:ILE:O	2.33	0.47
1:B:64:LEU:HD13	1:B:115:TRP:HH2	1.79	0.47
1:C:93:VAL:CG2	1:C:104:LEU:HD22	2.44	0.47
1:B:85:ILE:CD1	1:B:149:MET:HE3	2.40	0.47
1:D:6:LYS:O	1:D:7:LYS:HG2	2.13	0.47
2:G:3:BGC:C3	2:G:4:BGC:C2	2.83	0.47
1:A:14:LEU:HB3	1:A:93:VAL:HG22	1.96	0.47
1:C:30:ARG:HD2	1:C:103:TRP:HE1	1.75	0.47
1:A:26:GLY:HA3	3:A:188:HOH:O	2.14	0.47
1:C:79:GLU:H	1:C:79:GLU:HG2	1.52	0.47
1:D:39:ARG:NH1	1:D:39:ARG:CG	2.75	0.46
1:B:98:GLU:HA	1:B:99:PRO:HA	1.69	0.46
1:C:60:LEU:HD22	1:C:115:TRP:CE3	2.50	0.46
1:C:142:ARG:HA	1:C:142:ARG:HD3	1.70	0.46
1:B:103:TRP:O	1:B:106:PRO:HD2	2.15	0.46
1:C:130:ARG:HG3	1:C:131:ASP:N	2.30	0.46
1:D:50:CYS:SG	1:D:59:GLU:HG3	2.56	0.46
1:C:66:LEU:HD13	2:F:5[A]:BGC:O2	2.16	0.46
1:D:128:VAL:HA	1:D:148:TYR:O	2.15	0.46
1:B:66:LEU:HD12	2:F:2[A]:BGC:C2	2.43	0.46
1:A:137:LEU:HA	1:A:140:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ALA:HB3	1:B:123:PHE:CE1	2.51	0.45
1:C:83:LEU:HB3	1:C:149:MET:HB3	1.99	0.45
1:C:97:GLY:CA	1:C:98:GLU:OE2	2.64	0.45
2:G:3:BGC:C3	2:G:4:BGC:H2	2.39	0.45
1:B:41:MET:CE	1:B:107:VAL:HG11	2.40	0.45
1:B:109:GLU:HA	1:B:147:MET:CE	2.46	0.45
1:C:7:LYS:CB	1:C:8:PRO:CD	2.86	0.45
1:D:22:ASP:OD1	1:D:30:ARG:HD3	2.17	0.45
1:D:137:LEU:HD12	1:D:137:LEU:N	2.28	0.45
1:B:45:ILE:HG22	1:C:45:ILE:HG22	1.99	0.44
1:C:102:THR:HG23	1:C:102:THR:O	2.16	0.44
1:D:80:ASP:O	1:D:81:GLN:HB2	2.16	0.44
1:A:22:ASP:OD1	1:A:30:ARG:CD	2.62	0.44
1:C:113:GLY:O	1:C:117:THR:HB	2.18	0.44
1:A:4:PHE:N	1:A:4:PHE:CD2	2.85	0.44
1:A:130:ARG:HG3	1:A:130:ARG:O	2.17	0.44
1:B:122:ALA:HB3	1:B:123:PHE:CD1	2.52	0.44
1:C:62:ALA:HA	2:F:1[B]:BGC:HC	1.82	0.44
1:B:79:GLU:HG2	1:B:80:ASP:OD1	2.18	0.44
1:A:83:LEU:HB3	1:A:149:MET:HB3	2.00	0.44
1:C:27:ILE:HG12	1:C:98:GLU:OE1	2.18	0.43
1:D:93:VAL:HG23	1:D:93:VAL:O	2.18	0.43
2:F:3[A]:BGC:C3	2:F:4[A]:BGC:C2	2.78	0.43
2:G:4:BGC:H6C2	2:G:5:BGC:O6	2.19	0.43
1:D:18:SER:HA	1:D:103:TRP:CZ2	2.53	0.43
1:B:79:GLU:CD	1:B:79:GLU:H	2.21	0.43
1:B:80:ASP:OD1	1:B:80:ASP:N	2.52	0.43
1:A:127:VAL:HG12	1:A:128:VAL:H	1.83	0.43
1:C:104:LEU:HD12	1:C:107:VAL:HG21	2.01	0.43
1:A:127:VAL:O	1:A:149:MET:HA	2.19	0.43
2:F:4[A]:BGC:H6C2	2:F:5[A]:BGC:O5	2.19	0.43
1:A:18:SER:HA	1:A:103:TRP:CZ2	2.54	0.43
1:B:155:ALA:HB1	1:B:158:HIS:ND1	2.28	0.43
1:C:87:HIS:C	1:C:87:HIS:CD2	2.92	0.43
1:A:76:LEU:HD11	1:A:81:GLN:HE22	1.84	0.43
1:C:12:LEU:O	1:C:16:THR:HG23	2.19	0.42
1:C:50:CYS:SG	1:C:56:LEU:HA	2.59	0.42
1:C:5:GLU:O	1:C:7:LYS:CE	2.68	0.42
1:D:127:VAL:HG12	1:D:128:VAL:N	2.33	0.42
1:C:15:GLN:NE2	2:G:5:BGC:O3	2.53	0.42
1:C:32:GLU:OE1	1:C:35:ARG:NH1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ASP:OD1	1:B:30:ARG:HD3	2.19	0.42
1:A:57:GLN:HG2	1:A:61:ASN:ND2	2.34	0.42
1:C:63:LEU:HD12	1:C:63:LEU:HA	1.91	0.42
1:D:134:ALA:O	1:D:135:GLU:HB3	2.19	0.42
1:D:46:MET:HB2	1:D:47:PRO:HD2	2.02	0.42
1:D:60:LEU:HD22	1:D:115:TRP:CE3	2.55	0.42
1:B:156:THR:CA	1:B:158:HIS:HD2	2.33	0.41
1:C:46:MET:HB3	3:C:185:HOH:O	2.19	0.41
1:C:80:ASP:OD1	1:C:80:ASP:C	2.58	0.41
1:C:93:VAL:HG22	1:C:104:LEU:HD22	2.02	0.41
1:A:74:LEU:HD12	1:A:85:ILE:HG12	2.01	0.41
3:B:166:HOH:O	1:C:44:ARG:HD2	2.20	0.41
1:C:102:THR:O	1:C:102:THR:CG2	2.68	0.41
1:D:106:PRO:HD2	3:D:200:HOH:O	2.19	0.41
1:D:132:VAL:O	1:D:135:GLU:CA	2.68	0.41
1:B:156:THR:CA	1:B:158:HIS:CD2	3.04	0.41
2:F:1[B]:BGC:C6	2:F:2[B]:BGC:C1	2.95	0.41
2:F:4[B]:BGC:H6C2	2:F:5[B]:BGC:O5	2.21	0.41
1:C:5:GLU:O	1:C:7:LYS:HE3	2.21	0.41
1:B:63:LEU:HD12	1:B:63:LEU:HA	1.97	0.40
1:C:80:ASP:O	1:C:81:GLN:HB2	2.21	0.40
1:C:61:ASN:HA	3:C:270:HOH:O	2.20	0.40
1:A:57:GLN:HG2	1:A:61:ASN:HD21	1.85	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	146/162 (90%)	130 (89%)	14 (10%)	2 (1%)	11	43
1	B	156/162 (96%)	147 (94%)	7 (4%)	2 (1%)	12	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	157/162 (97%)	143 (91%)	12 (8%)	2 (1%)	12	45
1	D	146/162 (90%)	138 (94%)	5 (3%)	3 (2%)	7	33
All	All	605/648 (93%)	558 (92%)	38 (6%)	9 (2%)	10	42

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	121	GLY
1	C	122	ALA
1	D	7	LYS
1	D	70	GLY
1	C	120	ALA
1	D	120	ALA
1	B	7	LYS
1	A	7	LYS
1	A	124	GLY

### 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	127/140 (91%)	102 (80%)	25 (20%)	1	7
1	B	136/140 (97%)	113 (83%)	23 (17%)	2	11
1	C	137/140 (98%)	112 (82%)	25 (18%)	1	9
1	D	127/140 (91%)	103 (81%)	24 (19%)	1	8
All	All	527/560 (94%)	430 (82%)	97 (18%)	1	9

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	14	LEU
1	A	16	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	19	TRP
1	A	23	ASP
1	A	29	VAL
1	A	32	GLU
1	A	33	LEU
1	A	46	MET
1	A	53	VAL
1	A	63	LEU
1	A	74	LEU
1	A	75	GLU
1	A	77	LEU
1	A	81	GLN
1	A	93	VAL
1	A	102	THR
1	A	104	LEU
1	A	119	GLN
1	A	128	VAL
1	A	130	ARG
1	A	136	ASP
1	A	138	ASN
1	A	149	MET
1	A	150	ARG
1	B	4	PHE
1	B	9	ASP
1	B	14	LEU
1	B	16	THR
1	B	23	ASP
1	B	24	GLN
1	B	27	ILE
1	B	34	LEU
1	B	39	ARG
1	B	46	MET
1	B	51	GLN
1	B	63	LEU
1	B	64	LEU
1	B	80	ASP
1	B	84	ARG
1	B	104	LEU
1	B	125	ASP
1	B	132	VAL
1	B	133	ASP
1	B	136	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	152	ARG
1	B	157	HIS
1	B	158	HIS
1	C	23	ASP
1	C	25	VAL
1	C	34	LEU
1	C	39	ARG
1	C	46	MET
1	C	51	GLN
1	C	63	LEU
1	C	77	LEU
1	C	79	GLU
1	C	80	ASP
1	C	83	LEU
1	C	98	GLU
1	C	102	THR
1	C	104	LEU
1	C	108	LEU
1	C	125	ASP
1	C	129	THR
1	C	130	ARG
1	C	142	ARG
1	C	150	ARG
1	C	152	ARG
1	C	157	HIS
1	C	158	HIS
1	C	160	HIS
1	C	161	HIS
1	D	4	PHE
1	D	6	LYS
1	D	9	ASP
1	D	11	THR
1	D	12	LEU
1	D	34	LEU
1	D	39	ARG
1	D	51	GLN
1	D	53	VAL
1	D	63	LEU
1	D	66	LEU
1	D	74	LEU
1	D	76	LEU
1	D	80	ASP

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Mol	Chain	Res	Type
1	D	83	LEU
1	D	98	GLU
1	D	114	ARG
1	D	123	PHE
1	D	130	ARG
1	D	136	ASP
1	D	137	LEU
1	D	138	ASN
1	D	142	ARG
1	D	149	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	81	GLN
1	A	138	ASN
1	B	51	GLN
1	B	157	HIS
1	B	158	HIS
1	C	15	GLN
1	C	119	GLN
1	C	158	HIS
1	D	57	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](#)

20 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	E	1	2	12,12,12	0.60	0	17,17,17	1.10	1 (5%)
2	BGC	E	2	2	11,11,12	0.37	0	15,15,17	0.76	0
2	BGC	E	3	2	11,11,12	0.53	0	15,15,17	1.01	2 (13%)
2	BGC	E	4	2	11,11,12	0.52	0	15,15,17	1.53	4 (26%)
2	BGC	E	5	2	11,11,12	0.40	0	15,15,17	1.69	5 (33%)
2	BGC	F	1[A]	2	12,12,12	0.57	0	17,17,17	1.12	2 (11%)
2	BGC	F	1[B]	2	12,12,12	0.57	0	17,17,17	1.09	1 (5%)
2	BGC	F	2[A]	2	11,11,12	0.34	0	15,15,17	0.80	0
2	BGC	F	2[B]	2	11,11,12	0.36	0	15,15,17	0.83	0
2	BGC	F	3[A]	2	11,11,12	0.54	0	15,15,17	0.94	1 (6%)
2	BGC	F	3[B]	2	11,11,12	0.51	0	15,15,17	0.99	1 (6%)
2	BGC	F	4[A]	2	11,11,12	0.74	0	15,15,17	1.85	5 (33%)
2	BGC	F	4[B]	2	11,11,12	0.70	0	15,15,17	1.89	6 (40%)
2	BGC	F	5[A]	2	11,11,12	0.33	0	15,15,17	1.59	4 (26%)
2	BGC	F	5[B]	2	11,11,12	0.29	0	15,15,17	1.72	5 (33%)
2	BGC	G	1	2	12,12,12	0.67	0	17,17,17	1.22	2 (11%)
2	BGC	G	2	2	11,11,12	0.38	0	15,15,17	0.85	0
2	BGC	G	3	2	11,11,12	0.49	0	15,15,17	0.97	1 (6%)
2	BGC	G	4	2	11,11,12	0.62	0	15,15,17	1.51	5 (33%)
2	BGC	G	5	2	11,11,12	0.63	0	15,15,17	1.68	3 (20%)

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	E	1	2	-	2/2/22/22	0/1/1/1
2	BGC	E	2	2	-	2/2/19/22	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
2	BGC	E	5	2	-	2/2/19/22	0/1/1/1
2	BGC	F	1[A]	2	-	2/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	F	1[B]	2	-	2/2/22/22	0/1/1/1
2	BGC	F	2[A]	2	-	2/2/19/22	0/1/1/1
2	BGC	F	2[B]	2	-	2/2/19/22	0/1/1/1
2	BGC	F	3[A]	2	-	2/2/19/22	0/1/1/1
2	BGC	F	3[B]	2	-	2/2/19/22	0/1/1/1
2	BGC	F	4[A]	2	-	2/2/19/22	0/1/1/1
2	BGC	F	4[B]	2	-	2/2/19/22	0/1/1/1
2	BGC	F	5[A]	2	-	2/2/19/22	0/1/1/1
2	BGC	F	5[B]	2	-	2/2/19/22	0/1/1/1
2	BGC	G	1	2	-	2/2/22/22	0/1/1/1
2	BGC	G	2	2	-	2/2/19/22	0/1/1/1
2	BGC	G	3	2	-	0/2/19/22	0/1/1/1
2	BGC	G	4	2	-	2/2/19/22	0/1/1/1
2	BGC	G	5	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5	BGC	C2-C3-C4	3.71	117.32	110.89
2	G	5	BGC	C2-C3-C4	3.61	117.14	110.89
2	F	4[B]	BGC	O5-C5-C6	-3.59	101.57	107.20
2	F	4[A]	BGC	O5-C5-C6	-3.38	101.91	107.20
2	F	4[B]	BGC	O5-C1-C2	-3.36	105.59	110.77
2	F	4[A]	BGC	O5-C1-C2	-3.23	105.79	110.77
2	F	5[B]	BGC	O5-C1-C2	-3.16	105.89	110.77
2	G	5	BGC	O5-C5-C6	3.02	111.93	107.20
2	F	5[B]	BGC	C1-O5-C5	3.00	116.25	112.19
2	F	4[A]	BGC	C2-C3-C4	2.86	115.84	110.89
2	G	1	BGC	O4-C4-C5	2.83	116.33	109.30
2	F	5[A]	BGC	C2-C3-C4	2.83	115.79	110.89
2	F	5[A]	BGC	O5-C1-C2	-2.70	106.60	110.77
2	F	3[B]	BGC	C3-C4-C5	2.63	114.93	110.24
2	E	1	BGC	O4-C4-C5	2.62	115.80	109.30
2	F	4[B]	BGC	O4-C4-C5	2.58	115.71	109.30
2	G	5	BGC	O5-C1-C2	-2.58	106.79	110.77
2	F	1[B]	BGC	O4-C4-C5	2.58	115.69	109.30
2	F	1[A]	BGC	O4-C4-C5	2.57	115.68	109.30
2	F	4[A]	BGC	O4-C4-C5	2.47	115.44	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	4	BGC	C3-C4-C5	2.46	114.62	110.24
2	E	5	BGC	O5-C1-C2	-2.45	106.98	110.77
2	F	5[B]	BGC	C2-C3-C4	2.42	115.08	110.89
2	E	5	BGC	O3-C3-C2	-2.39	105.41	109.99
2	F	5[B]	BGC	C3-C4-C5	2.36	114.45	110.24
2	E	4	BGC	C3-C4-C5	2.35	114.44	110.24
2	F	3[A]	BGC	C3-C4-C5	2.35	114.43	110.24
2	G	4	BGC	O5-C1-C2	-2.32	107.18	110.77
2	E	5	BGC	O5-C5-C6	2.31	110.83	107.20
2	F	4[B]	BGC	C3-C4-C5	2.29	114.33	110.24
2	F	4[B]	BGC	C2-C3-C4	2.28	114.84	110.89
2	F	5[B]	BGC	O5-C5-C6	2.28	110.77	107.20
2	F	5[A]	BGC	C3-C4-C5	2.28	114.30	110.24
2	F	5[A]	BGC	O5-C5-C6	2.27	110.76	107.20
2	G	4	BGC	O2-C2-C3	-2.27	105.60	110.14
2	G	3	BGC	C3-C4-C5	2.26	114.28	110.24
2	E	4	BGC	O5-C1-C2	-2.26	107.29	110.77
2	E	3	BGC	O5-C5-C6	2.23	110.70	107.20
2	G	1	BGC	C4-C3-C2	2.18	114.63	110.82
2	F	4[B]	BGC	O2-C2-C3	-2.17	105.79	110.14
2	G	4	BGC	O4-C4-C5	2.17	114.68	109.30
2	E	3	BGC	C3-C4-C5	2.13	114.04	110.24
2	F	4[A]	BGC	C3-C4-C5	2.13	114.03	110.24
2	E	5	BGC	C3-C4-C5	2.11	114.01	110.24
2	F	1[A]	BGC	C4-C3-C2	2.11	114.50	110.82
2	E	4	BGC	O2-C2-C3	-2.08	105.97	110.14
2	G	4	BGC	C2-C3-C4	2.05	114.44	110.89
2	E	4	BGC	O4-C4-C5	2.02	114.32	109.30

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	5	BGC	O5-C5-C6-O6
2	F	5[B]	BGC	O5-C5-C6-O6
2	G	4	BGC	O5-C5-C6-O6
2	G	5	BGC	O5-C5-C6-O6
2	F	5[A]	BGC	O5-C5-C6-O6
2	F	2[B]	BGC	C4-C5-C6-O6
2	G	2	BGC	C4-C5-C6-O6
2	F	2[A]	BGC	C4-C5-C6-O6
2	F	5[B]	BGC	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	E	2	BGC	C4-C5-C6-O6
2	F	5[A]	BGC	C4-C5-C6-O6
2	E	5	BGC	C4-C5-C6-O6
2	E	1	BGC	O5-C5-C6-O6
2	G	5	BGC	C4-C5-C6-O6
2	F	2[B]	BGC	O5-C5-C6-O6
2	G	2	BGC	O5-C5-C6-O6
2	E	1	BGC	C4-C5-C6-O6
2	F	2[A]	BGC	O5-C5-C6-O6
2	G	4	BGC	C4-C5-C6-O6
2	E	2	BGC	O5-C5-C6-O6
2	G	1	BGC	C4-C5-C6-O6
2	G	1	BGC	O5-C5-C6-O6
2	F	3[A]	BGC	C4-C5-C6-O6
2	F	4[B]	BGC	C4-C5-C6-O6
2	F	3[B]	BGC	C4-C5-C6-O6
2	F	3[A]	BGC	O5-C5-C6-O6
2	F	4[B]	BGC	O5-C5-C6-O6
2	F	1[A]	BGC	C4-C5-C6-O6
2	F	1[B]	BGC	C4-C5-C6-O6
2	F	1[A]	BGC	O5-C5-C6-O6
2	F	3[B]	BGC	O5-C5-C6-O6
2	F	4[A]	BGC	C4-C5-C6-O6
2	F	1[B]	BGC	O5-C5-C6-O6
2	F	4[A]	BGC	O5-C5-C6-O6

There are no ring outliers.

20 monomers are involved in 58 short contacts:

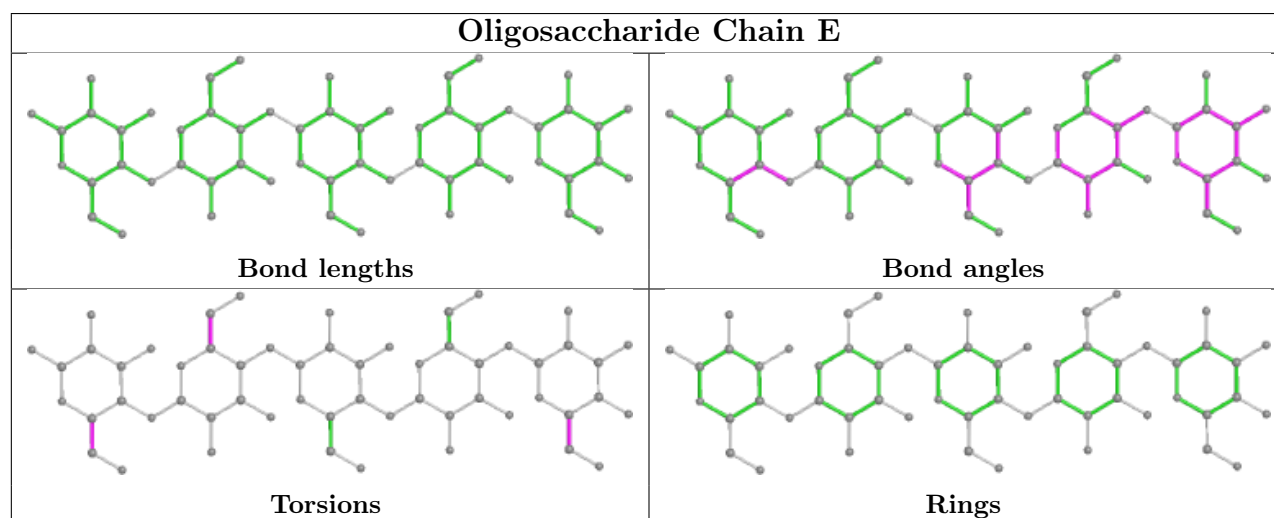
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	5	BGC	5	0
2	F	3[B]	BGC	4	0
2	F	5[B]	BGC	4	0
2	F	4[B]	BGC	10	0
2	G	4	BGC	9	0
2	E	4	BGC	4	0
2	F	3[A]	BGC	5	0
2	F	5[A]	BGC	5	0
2	F	4[A]	BGC	8	0
2	F	2[B]	BGC	2	0
2	F	1[B]	BGC	4	0
2	F	2[A]	BGC	4	0

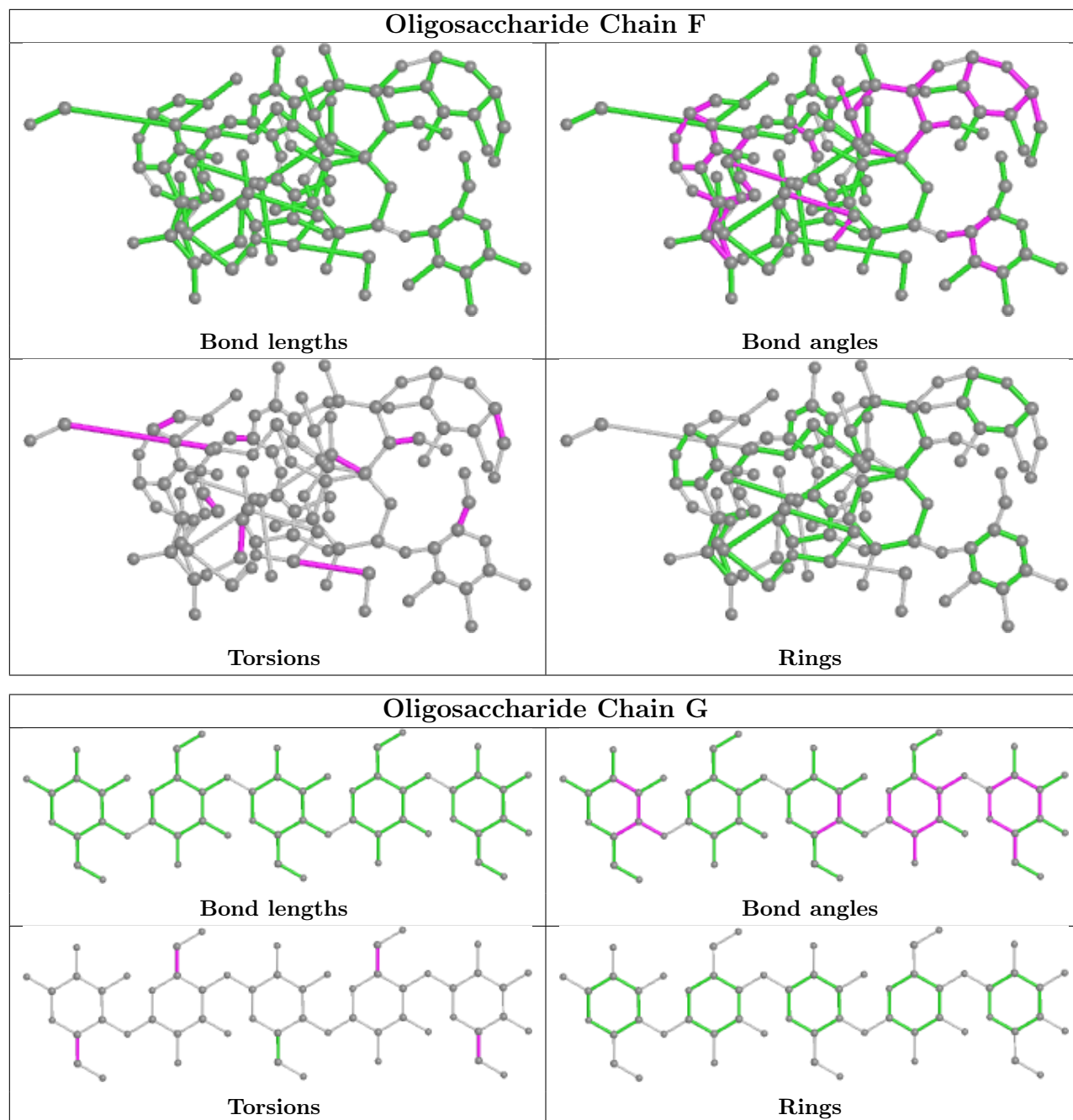
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1[A]	BGC	2	0
2	E	5	BGC	4	0
2	G	3	BGC	5	0
2	E	3	BGC	4	0
2	E	2	BGC	1	0
2	G	1	BGC	2	0
2	E	1	BGC	2	0
2	G	2	BGC	1	0

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

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	148/162 (91%)	-0.16	9 (6%) 21 7	30, 49, 108, 156	0
1	B	158/162 (97%)	-0.17	8 (5%) 28 10	32, 47, 92, 146	0
1	C	159/162 (98%)	-0.19	6 (3%) 40 16	28, 47, 94, 139	0
1	D	148/162 (91%)	-0.09	10 (6%) 17 5	29, 45, 107, 157	0
All	All	613/648 (94%)	-0.15	33 (5%) 25 9	28, 47, 102, 157	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	GLU	6.3
1	D	120	ALA	5.5
1	B	4	PHE	5.4
1	C	4	PHE	4.7
1	D	134	ALA	4.4
1	D	133	ASP	4.4
1	D	135	GLU	4.3
1	C	5	GLU	4.3
1	C	138	ASN	4.3
1	A	134	ALA	4.2
1	B	134	ALA	4.0
1	D	136	ASP	4.0
1	A	135	GLU	3.9
1	C	135	GLU	3.5
1	B	135	GLU	3.4
1	A	4	PHE	3.4
1	A	138	ASN	3.3
1	A	79	GLU	3.2
1	A	125	ASP	3.0
1	A	5	GLU	2.9
1	C	134	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	5	GLU	2.8
1	B	81	GLN	2.8
1	D	138	ASN	2.7
1	D	4	PHE	2.7
1	D	122	ALA	2.7
1	B	161	HIS	2.7
1	A	133	ASP	2.7
1	D	121	GLY	2.7
1	B	120	ALA	2.5
1	C	152	ARG	2.4
1	A	51	GLN	2.1
1	B	152	ARG	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.

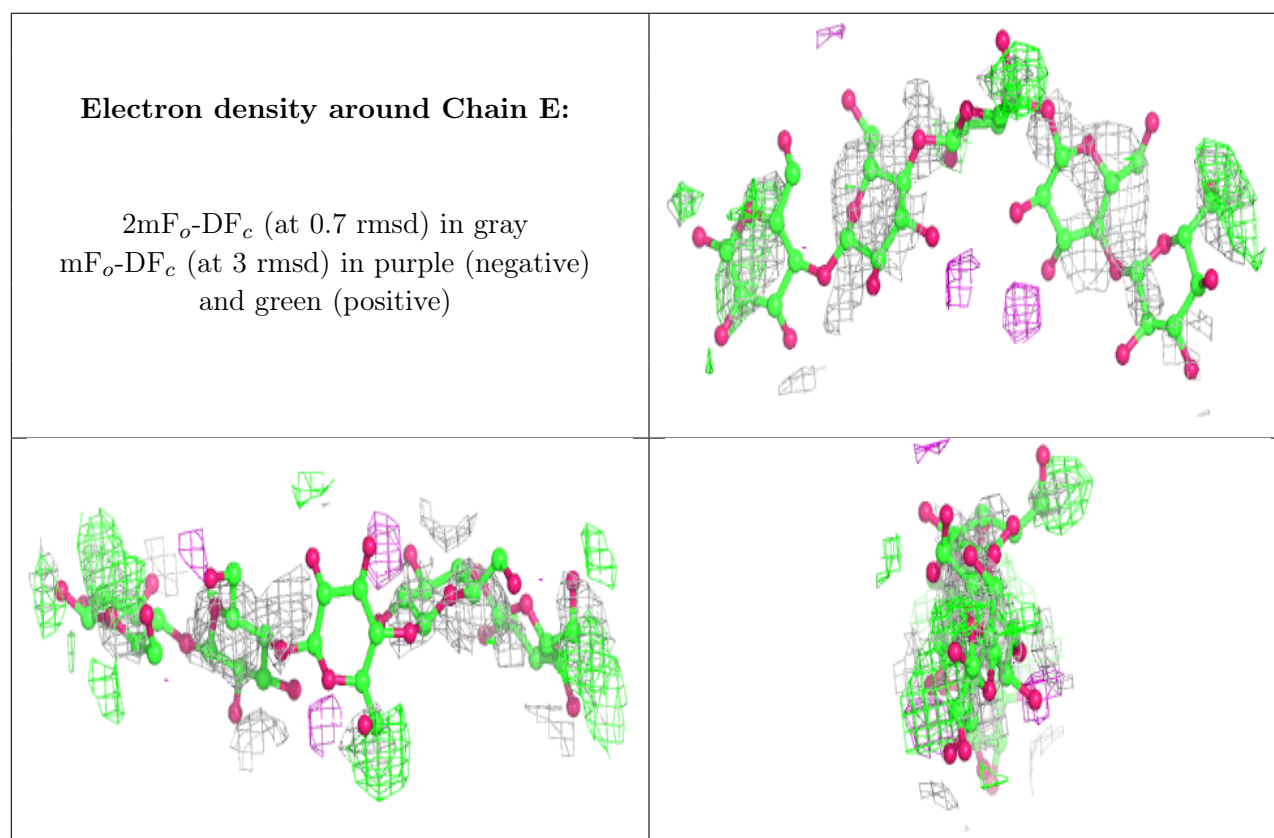
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BGC	E	3	11/12	0.34	0.71	54,55,55,55	11
2	BGC	E	1	12/12	0.36	0.70	54,55,55,55	12
2	BGC	F	1[A]	12/12	0.51	0.61	54,54,54,54	12
2	BGC	F	1[B]	12/12	0.51	0.61	55,55,55,56	12
2	BGC	F	3[A]	11/12	0.51	0.54	54,54,55,55	11
2	BGC	F	3[B]	11/12	0.51	0.54	54,54,55,55	11
2	BGC	G	3	11/12	0.54	0.57	54,54,55,55	11
2	BGC	F	5[B]	11/12	0.57	0.58	54,54,54,54	11
2	BGC	F	5[A]	11/12	0.57	0.58	54,54,54,54	11
2	BGC	G	1	12/12	0.59	0.51	55,55,56,56	12
2	BGC	G	2	11/12	0.60	0.48	55,55,55,56	11
2	BGC	E	5	11/12	0.67	0.48	55,55,55,55	11
2	BGC	G	4	11/12	0.68	0.54	53,53,54,54	11
2	BGC	E	2	11/12	0.71	0.40	54,55,55,55	11
2	BGC	F	4[A]	11/12	0.75	0.59	53,54,54,54	11

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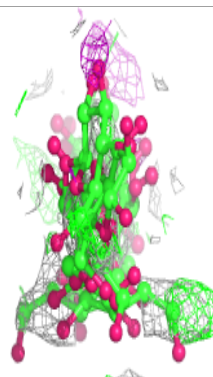
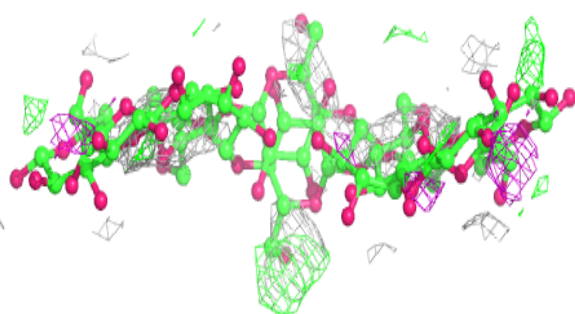
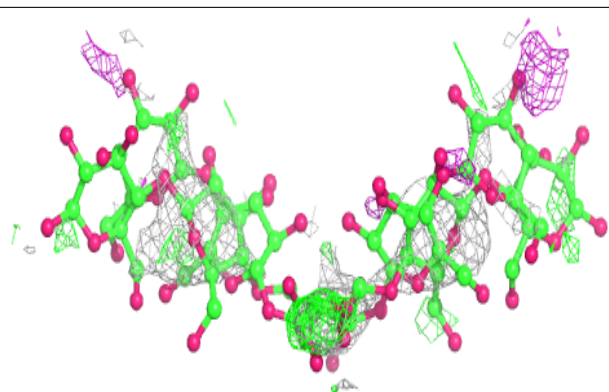
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BGC	F	4[B]	11/12	0.75	0.59	53,53,53,54	11
2	BGC	F	2[A]	11/12	0.75	0.54	54,54,55,55	11
2	BGC	F	2[B]	11/12	0.75	0.54	55,55,55,56	11
2	BGC	G	5	11/12	0.76	0.40	53,54,54,54	11
2	BGC	E	4	11/12	0.78	0.46	54,54,54,54	11

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.

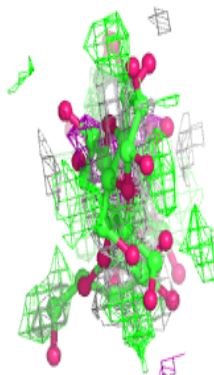
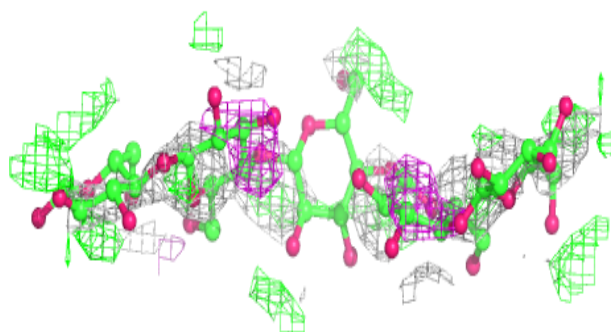
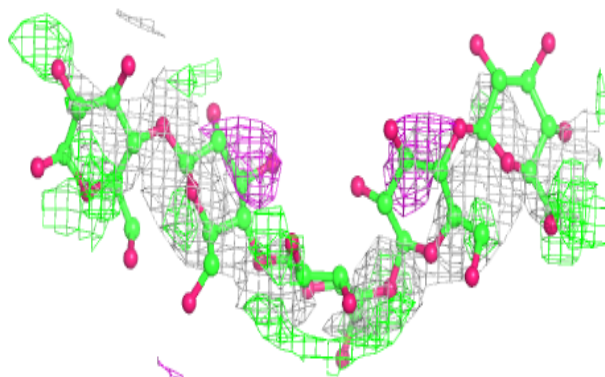


**Electron density around Chain F:**

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

**Electron density around Chain G:**

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





## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.