



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2021 – 03:02 PM EDT

PDB ID : 1DED  
Title : CRYSTAL STRUCTURE OF ALKALOPHILIC ASPARAGINE 233-REPLACED CYCLODEXTRIN GLUCANOTRANSFERASE COMPLEXED WITH AN INHIBITOR, ACARBOSE, AT 2.0 Å RESOLUTION  
Authors : Ishii, N.; Haga, K.; Yamane, K.; Harata, K.  
Deposited on : 1999-11-14  
Resolution : 2.00 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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 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 : 2.23.2  
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) : 2.23.2

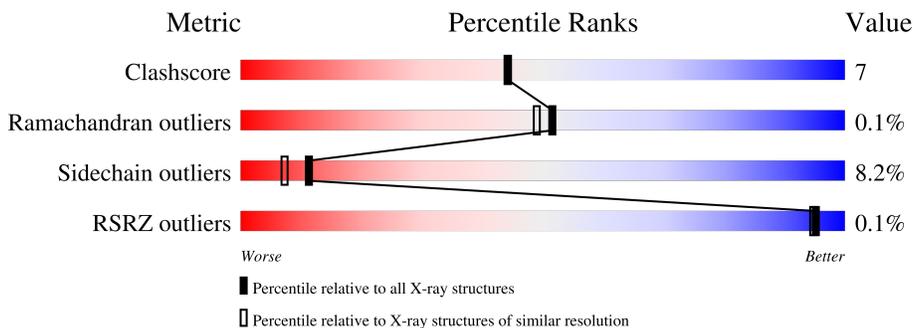
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
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	686	77% 18% . .
1	B	686	76% 20% . .
2	C	3	33% 67%
2	D	3	33% 67%
2	E	3	33% 67%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	C	2	-	-	-	X
2	GLC	D	2	-	-	-	X
2	AC1	D	3[A]	-	-	-	X
2	AC1	D	3[B]	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15555 atoms, of which 4040 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 CYCLODEXTRIN GLUCANOTRANSFERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	686	6505	3352	1195	905	1037	16	1195	0	0
1	B	686	6505	3352	1195	905	1037	16	1195	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	233	ASN	HIS	engineered mutation	UNP P05618
A	452	PRO	ARG	conflict	UNP P05618
A	454	GLY	ALA	conflict	UNP P05618
B	233	ASN	HIS	engineered mutation	UNP P05618
B	452	PRO	ARG	conflict	UNP P05618
B	454	GLY	ALA	conflict	UNP P05618

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4-[[{(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	C	3	88	25	44	1	18	44	1	0
2	D	3	88	25	44	1	18	44	1	0
2	E	3	88	25	44	1	18	44	1	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		

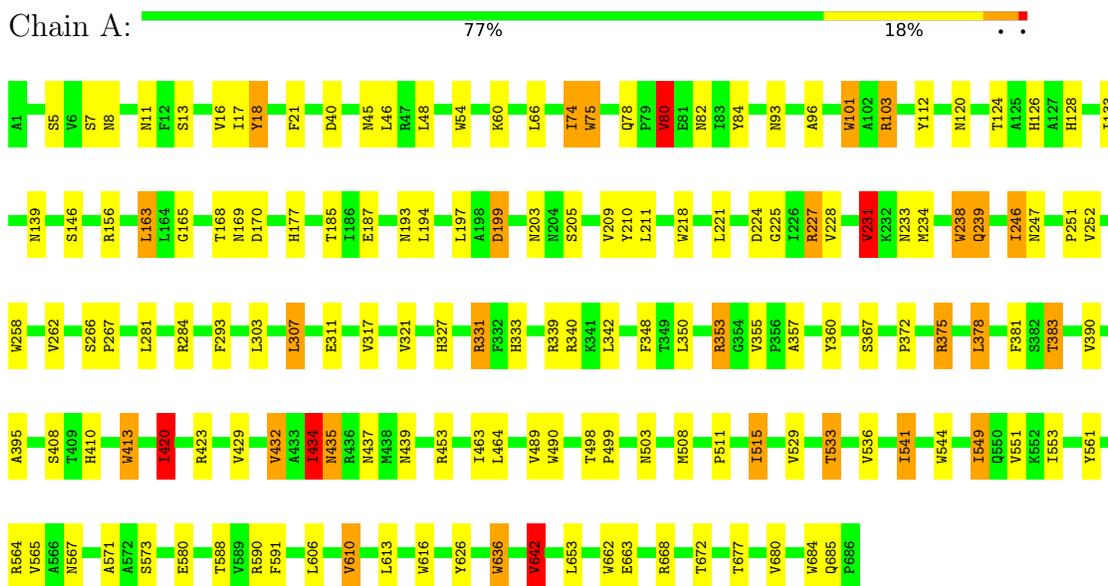
- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	405	Total	H	O	810	0
			1215	810	405		
4	B	354	Total	H	O	708	0
			1062	708	354		

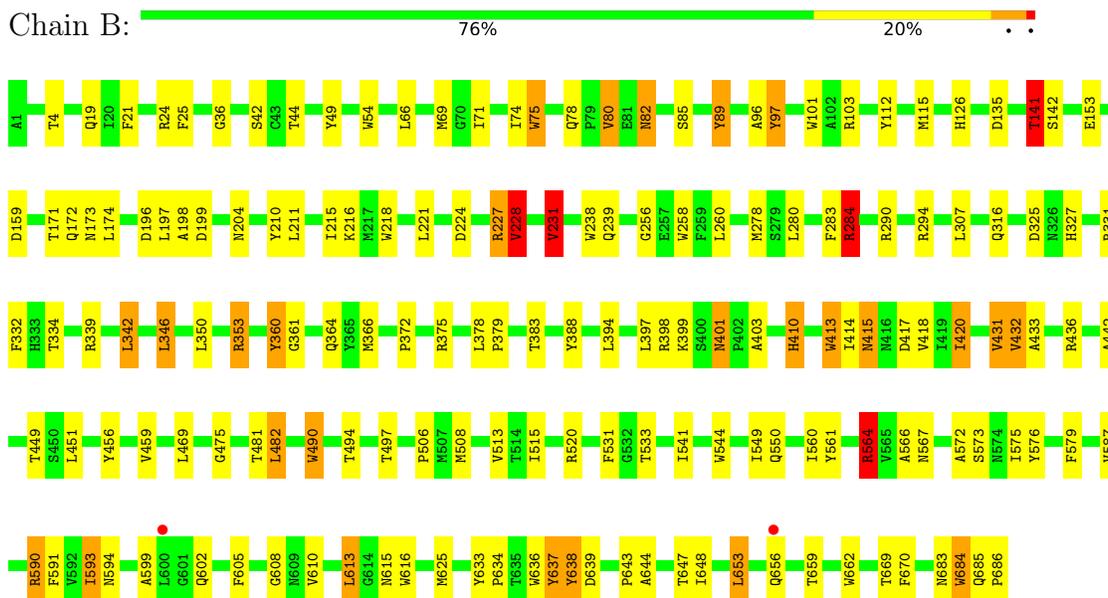
### 3 Residue-property plots

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: CYCLODEXTRIN GLUCANOTRANSFERASE



#### • Molecule 1: CYCLODEXTRIN GLUCANOTRANSFERASE



- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose-(1-4)- $\beta$ -D-glucopyranose

Chain C:  33% 67%

BGC1  
GLC2  
AC13

- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose-(1-4)- $\beta$ -D-glucopyranose

Chain D:  33% 67%

BGC1  
GLC2  
AC13

- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose-(1-4)- $\beta$ -D-glucopyranose

Chain E:  33% 67%

BGC1  
GLC2  
AC13

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.93Å 73.83Å 79.05Å 85.10° 105.40° 100.50°	Depositor
Resolution (Å)	10.00 – 2.00 20.27 – 1.85	Depositor EDS
% Data completeness (in resolution range)	62.3 (10.00-2.00) 80.8 (20.27-1.85)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.72 (at 1.85Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.163 , 0.222 0.201 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtrriage
Anisotropy	0.105	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 76.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15555	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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: GLC, CA, BGC, AC1

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	0.79	1/5443 (0.0%)	1.49	79/7425 (1.1%)
1	B	0.78	1/5443 (0.0%)	1.52	79/7425 (1.1%)
All	All	0.78	2/10886 (0.0%)	1.51	158/14850 (1.1%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	420	ILE	CA-CB	5.46	1.67	1.54
1	B	228	VAL	CA-CB	5.14	1.65	1.54

The worst 5 of 158 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	331	ARG	NE-CZ-NH2	-17.15	111.73	120.30
1	B	331	ARG	NE-CZ-NH1	12.86	126.73	120.30
1	B	227	ARG	NE-CZ-NH1	10.70	125.65	120.30
1	A	662	TRP	CD1-CG-CD2	9.93	114.25	106.30
1	A	590	ARG	NE-CZ-NH1	9.70	125.15	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	97	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	5310	1195	5049	69	0
1	B	5310	1195	5049	67	0
2	C	44	44	20	0	0
2	D	44	44	20	3	0
2	E	44	44	20	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	405	810	0	8	0
4	B	354	708	0	7	0
All	All	11515	4040	10158	138	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 7.

The worst 5 of 138 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:238:TRP:HD1	1:A:588:THR:HG21	1.50	0.77
1:A:231:VAL:HG22	1:A:239:GLN:HE22	1.51	0.76
1:A:293:PHE:HE2	1:A:434:ILE:HD11	1.49	0.76
1:A:434:ILE:HG21	4:A:3075:HOH:O	1.88	0.74
1:B:431:VAL:HG23	1:B:490:TRP:HE3	1.56	0.71

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	684/686 (100%)	662 (97%)	22 (3%)	0	100	100
1	B	684/686 (100%)	657 (96%)	25 (4%)	2 (0%)	41	37
All	All	1368/1372 (100%)	1319 (96%)	47 (3%)	2 (0%)	51	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	36	GLY
1	B	89	TYR

### 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	564/564 (100%)	518 (92%)	46 (8%)	11	7
1	B	564/564 (100%)	518 (92%)	46 (8%)	11	7
All	All	1128/1128 (100%)	1036 (92%)	92 (8%)	11	7

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	197	LEU
1	B	375	ARG
1	B	204	ASN
1	B	334	THR
1	B	415	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	578	ASN
1	B	416	ASN
1	A	646	GLN
1	B	548	GLN
1	B	364	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](#)

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	BGC	C	1	2	12,12,12	0.74	0	17,17,17	1.11	2 (11%)
2	GLC	C	2	2	11,11,12	1.08	1 (9%)	15,15,17	2.73	5 (33%)
2	BGC	D	1	2	12,12,12	1.32	1 (8%)	17,17,17	1.16	1 (5%)
2	GLC	D	2	2	11,11,12	1.62	2 (18%)	15,15,17	2.42	6 (40%)
2	BGC	E	1	2	12,12,12	0.97	1 (8%)	17,17,17	1.19	2 (11%)
2	GLC	E	2	2	11,11,12	0.97	0	15,15,17	1.32	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	1/2/19/22	0/1/1/1
2	BGC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	BGC	E	1	2	-	1/2/22/22	0/1/1/1
2	GLC	E	2	2	-	1/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	GLC	C2-C3	3.71	1.58	1.52
2	D	1	BGC	C4-C5	3.20	1.59	1.53
2	E	1	BGC	C4-C5	2.60	1.58	1.53
2	D	2	GLC	C1-C2	2.46	1.57	1.52
2	C	2	GLC	C4-C5	2.35	1.58	1.53

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	GLC	C1-O5-C5	7.82	122.79	112.19
2	D	2	GLC	C1-O5-C5	4.76	118.64	112.19
2	D	2	GLC	O5-C5-C6	4.09	113.62	107.20
2	D	2	GLC	O5-C5-C4	-3.43	102.49	110.83
2	C	2	GLC	O5-C5-C6	-3.41	101.85	107.20

There are no chirality outliers.

All (3) torsion outliers are listed below:

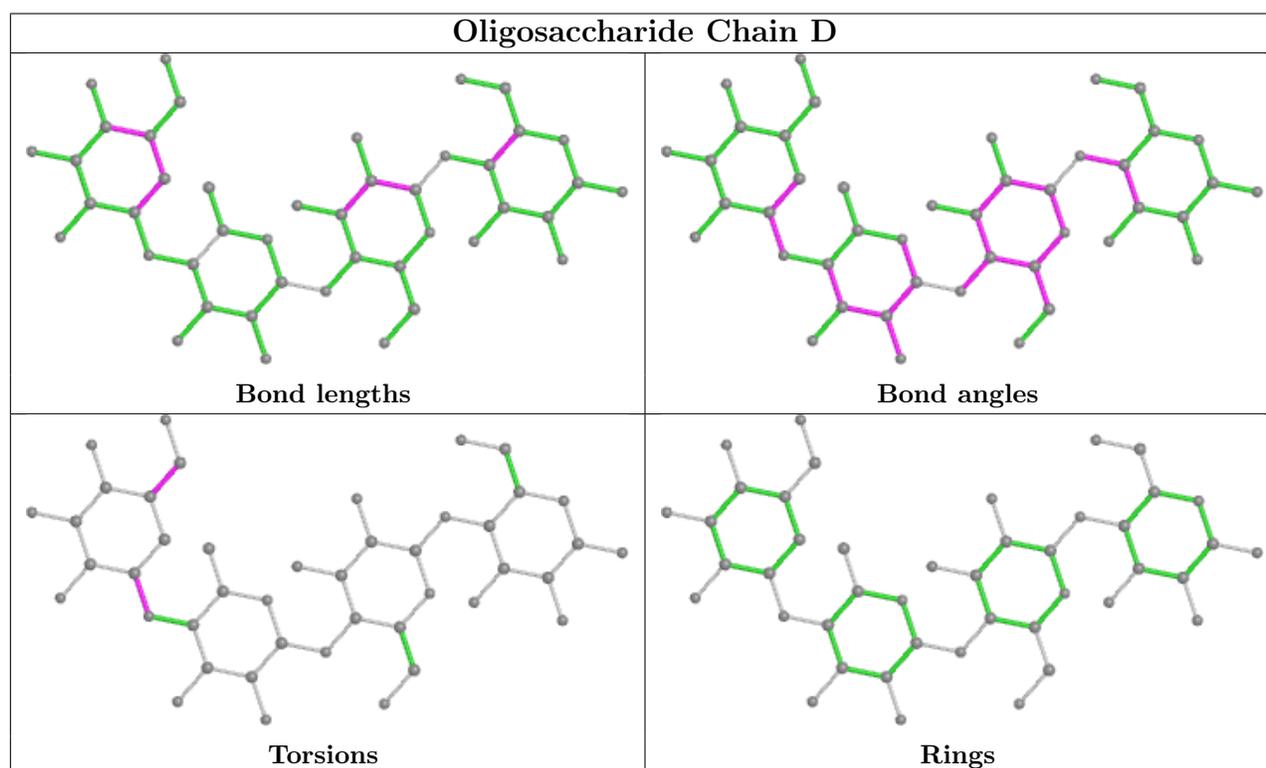
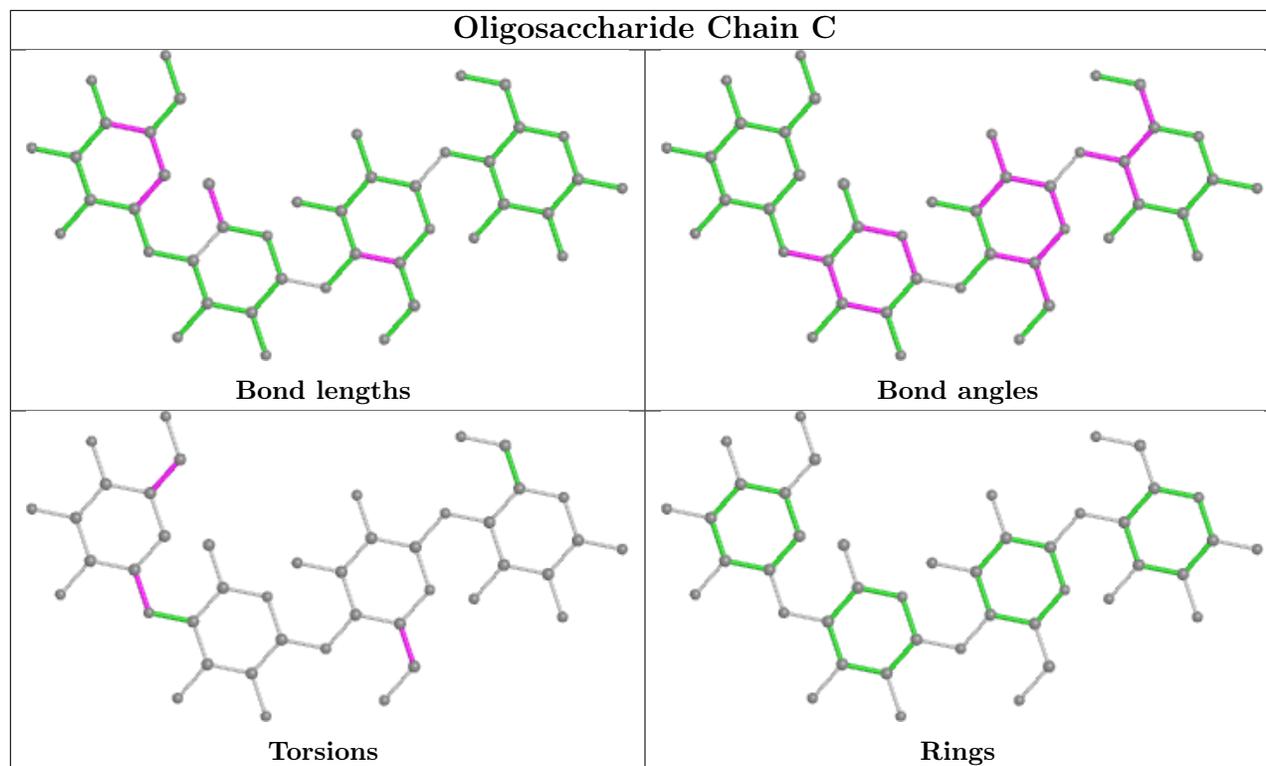
Mol	Chain	Res	Type	Atoms
2	E	2	GLC	O5-C5-C6-O6
2	E	1	BGC	O5-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6

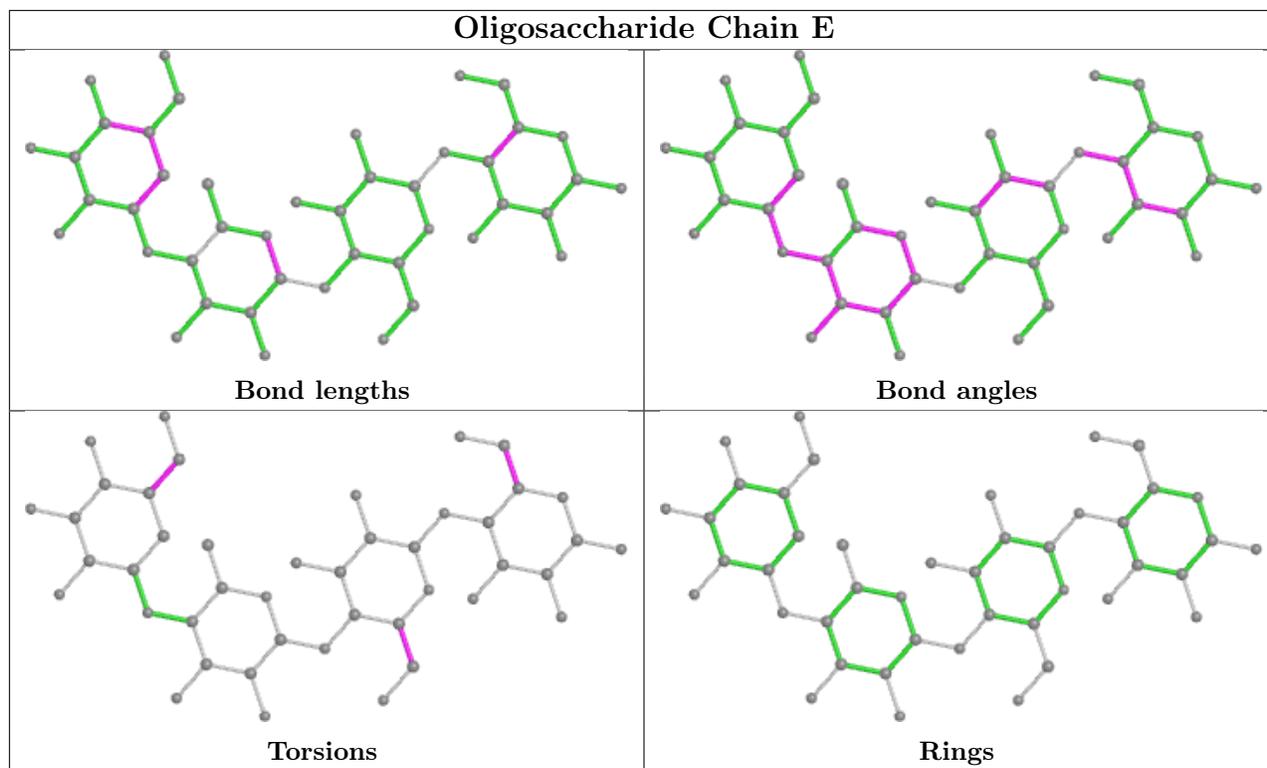
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	BGC	2	0
2	D	2	GLC	3	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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 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	686/686 (100%)	-0.36	0 100   100	6, 16, 32, 62	0
1	B	686/686 (100%)	-0.20	2 (0%) 94   93	6, 21, 44, 68	0
All	All	1372/1372 (100%)	-0.28	2 (0%) 95   95	6, 18, 40, 68	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	LEU	2.9
1	B	656	GLN	2.5

### 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.

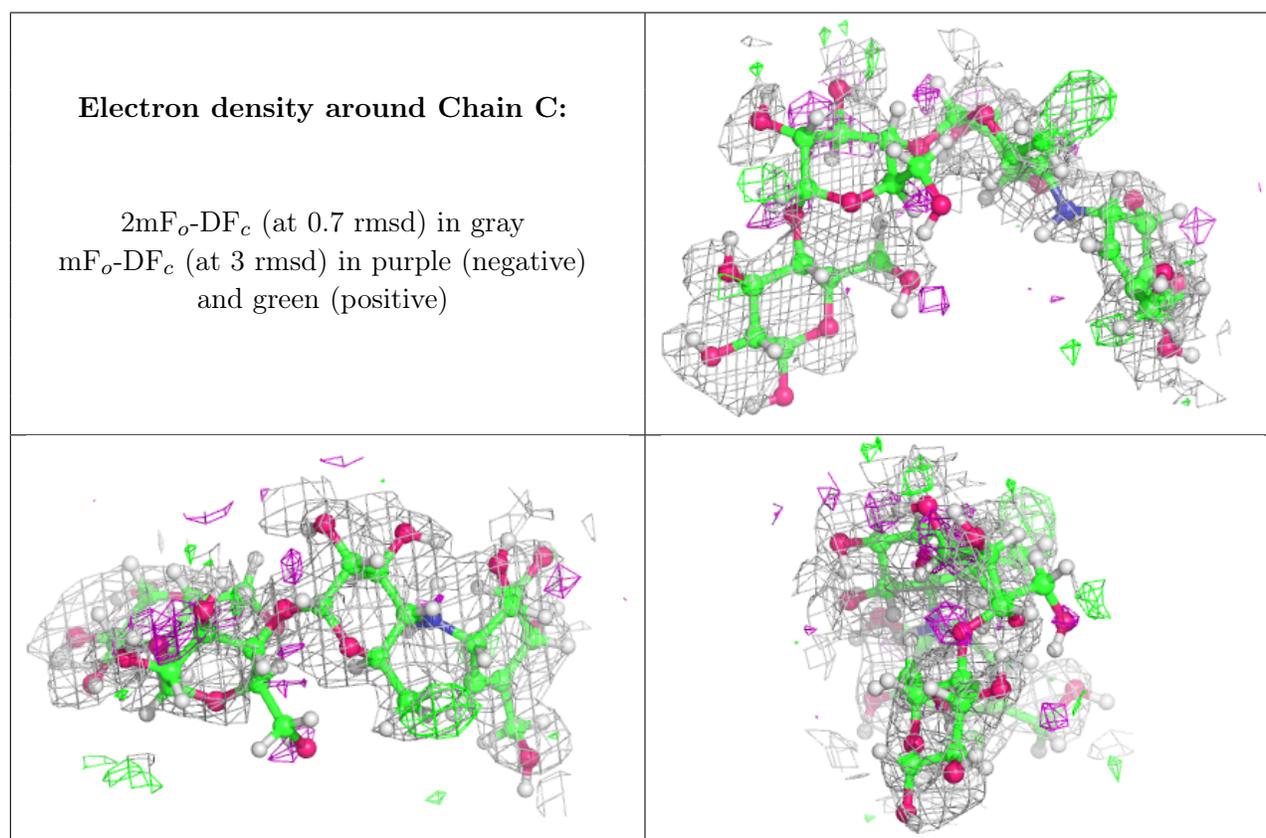
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	AC1	D	3[A]	21/22	0.43	0.67	0,0,101,102	22
2	AC1	D	3[B]	21/22	0.43	0.67	0,0,101,102	22
2	GLC	D	2	11/12	0.46	0.51	0,0,97,99	10
2	BGC	C	1	12/12	0.52	0.26	0,0,73,76	11
2	GLC	C	2	11/12	0.54	0.41	0,0,68,76	10
2	AC1	E	3[A]	21/22	0.61	0.23	0,0,59,60	22
2	AC1	E	3[B]	21/22	0.61	0.23	0,0,59,60	22

*Continued on next page...*

Continued from previous page...

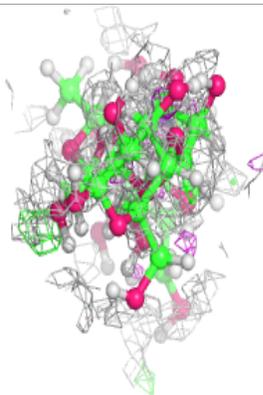
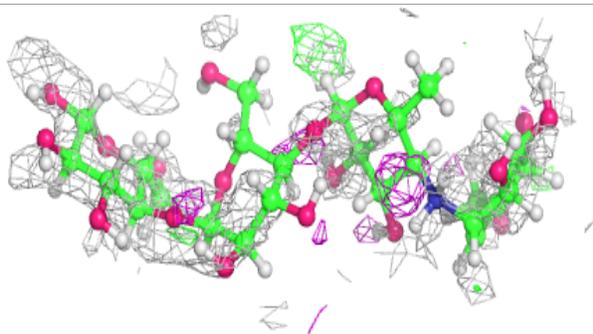
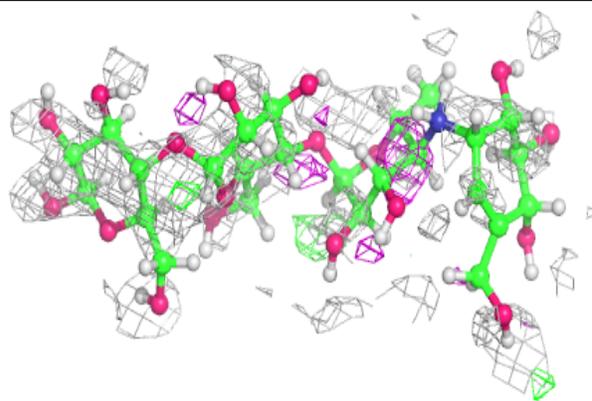
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BGC	E	1	12/12	0.63	0.25	0,0,71,73	11
2	AC1	C	3[A]	21/22	0.65	0.18	0,0,61,63	22
2	AC1	C	3[B]	21/22	0.65	0.18	0,0,61,63	22
2	BGC	D	1	12/12	0.68	0.37	0,0,92,94	11
2	GLC	E	2	11/12	0.79	0.23	0,0,62,68	10

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.

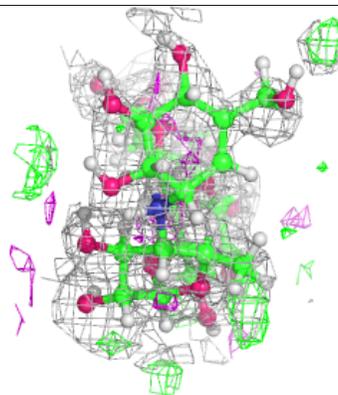
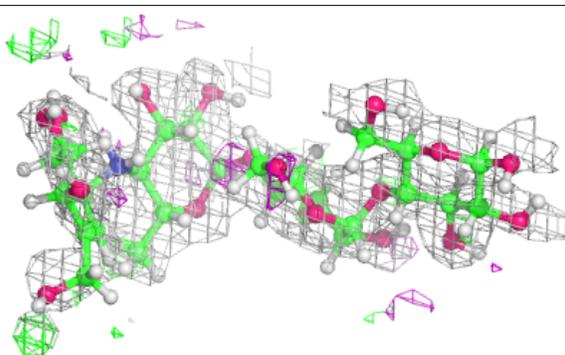
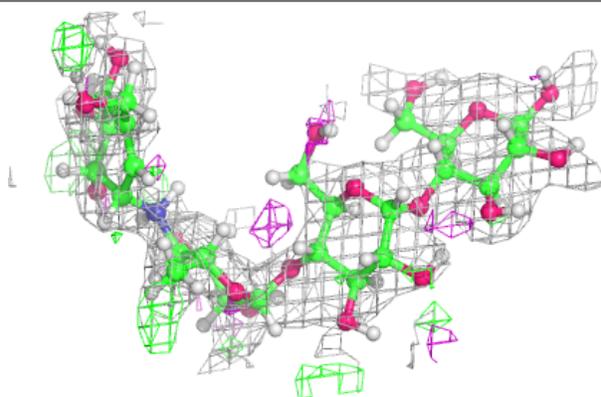


**Electron density around Chain D:**

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

**Electron density around Chain E:**

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



## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	B	5002	1/1	0.80	0.12	27,27,27,27	0
3	CA	A	5003	1/1	0.90	0.10	36,36,36,36	0
3	CA	B	5004	1/1	0.94	0.08	32,32,32,32	0
3	CA	A	5001	1/1	0.97	0.04	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.