W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jun 7, 2023 – 06:19 PM JST

PDB ID	:	8IUC
Title	:	Crystal structure of GH65 alpha-1,2-glucosidase from Flavobacterium johnsoniae in complex with isomaltose
Authors	:	Nakamura, S.; Miyazaki, T.
Deposited on	:	2023-03-24
Resolution	:	1.56 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.33
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)	:	2.33

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 1.56 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		0.223
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		1.1%
RSRZ outliers		3.0%

Worse — Better

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
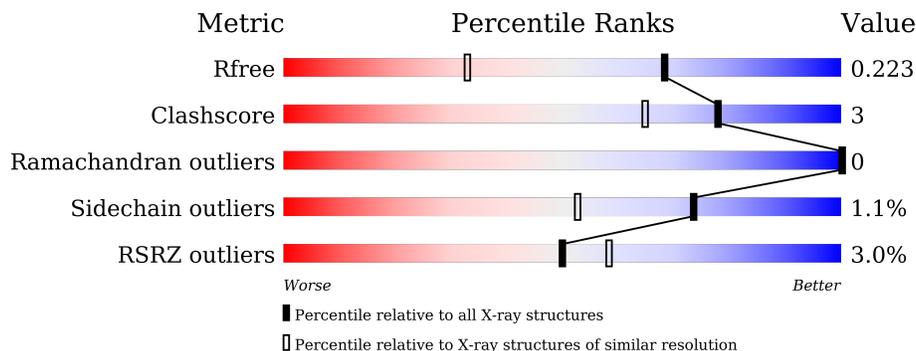
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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	678	2% / 90% / 7% •
1	B	678	5% / 87% / 10% •
1	C	678	% / 89% / 8% • •
2	D	2	50% / 50%
2	E	2	50% / 50%
2	F	2	50% / 50%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 33574 atoms, of which 15978 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 Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	659	Total	C	H	N	O	S	160	12	0
			10555	3392	5233	891	1017	22			
1	B	659	Total	C	H	N	O	S	159	12	0
			10545	3389	5229	889	1015	23			
1	C	659	Total	C	H	N	O	S	158	15	0
			10622	3411	5267	899	1022	23			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP A5FBJ5
A	5	GLY	-	expression tag	UNP A5FBJ5
A	6	SER	-	expression tag	UNP A5FBJ5
A	7	SER	-	expression tag	UNP A5FBJ5
A	8	HIS	-	expression tag	UNP A5FBJ5
A	9	HIS	-	expression tag	UNP A5FBJ5
A	10	HIS	-	expression tag	UNP A5FBJ5
A	11	HIS	-	expression tag	UNP A5FBJ5
A	12	HIS	-	expression tag	UNP A5FBJ5
A	13	HIS	-	expression tag	UNP A5FBJ5
A	14	SER	-	expression tag	UNP A5FBJ5
A	15	SER	-	expression tag	UNP A5FBJ5
A	16	GLY	-	expression tag	UNP A5FBJ5
A	17	LEU	-	expression tag	UNP A5FBJ5
A	18	VAL	-	expression tag	UNP A5FBJ5
A	19	PRO	-	expression tag	UNP A5FBJ5
A	20	ARG	-	expression tag	UNP A5FBJ5
A	21	GLY	-	expression tag	UNP A5FBJ5
A	22	SER	-	expression tag	UNP A5FBJ5
A	23	HIS	-	expression tag	UNP A5FBJ5
B	4	MET	-	initiating methionine	UNP A5FBJ5
B	5	GLY	-	expression tag	UNP A5FBJ5

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	SER	-	expression tag	UNP A5FBJ5
B	7	SER	-	expression tag	UNP A5FBJ5
B	8	HIS	-	expression tag	UNP A5FBJ5
B	9	HIS	-	expression tag	UNP A5FBJ5
B	10	HIS	-	expression tag	UNP A5FBJ5
B	11	HIS	-	expression tag	UNP A5FBJ5
B	12	HIS	-	expression tag	UNP A5FBJ5
B	13	HIS	-	expression tag	UNP A5FBJ5
B	14	SER	-	expression tag	UNP A5FBJ5
B	15	SER	-	expression tag	UNP A5FBJ5
B	16	GLY	-	expression tag	UNP A5FBJ5
B	17	LEU	-	expression tag	UNP A5FBJ5
B	18	VAL	-	expression tag	UNP A5FBJ5
B	19	PRO	-	expression tag	UNP A5FBJ5
B	20	ARG	-	expression tag	UNP A5FBJ5
B	21	GLY	-	expression tag	UNP A5FBJ5
B	22	SER	-	expression tag	UNP A5FBJ5
B	23	HIS	-	expression tag	UNP A5FBJ5
C	4	MET	-	initiating methionine	UNP A5FBJ5
C	5	GLY	-	expression tag	UNP A5FBJ5
C	6	SER	-	expression tag	UNP A5FBJ5
C	7	SER	-	expression tag	UNP A5FBJ5
C	8	HIS	-	expression tag	UNP A5FBJ5
C	9	HIS	-	expression tag	UNP A5FBJ5
C	10	HIS	-	expression tag	UNP A5FBJ5
C	11	HIS	-	expression tag	UNP A5FBJ5
C	12	HIS	-	expression tag	UNP A5FBJ5
C	13	HIS	-	expression tag	UNP A5FBJ5
C	14	SER	-	expression tag	UNP A5FBJ5
C	15	SER	-	expression tag	UNP A5FBJ5
C	16	GLY	-	expression tag	UNP A5FBJ5
C	17	LEU	-	expression tag	UNP A5FBJ5
C	18	VAL	-	expression tag	UNP A5FBJ5
C	19	PRO	-	expression tag	UNP A5FBJ5
C	20	ARG	-	expression tag	UNP A5FBJ5
C	21	GLY	-	expression tag	UNP A5FBJ5
C	22	SER	-	expression tag	UNP A5FBJ5
C	23	HIS	-	expression tag	UNP A5FBJ5

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-beta-D-glucopyranose.
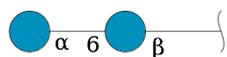
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	2	Total C H O				8	0	0
			46 12 23 11						
2	E	2	Total C H O				8	0	0
			46 12 23 11						
2	F	2	Total C H O				8	0	0
			46 12 23 11						

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
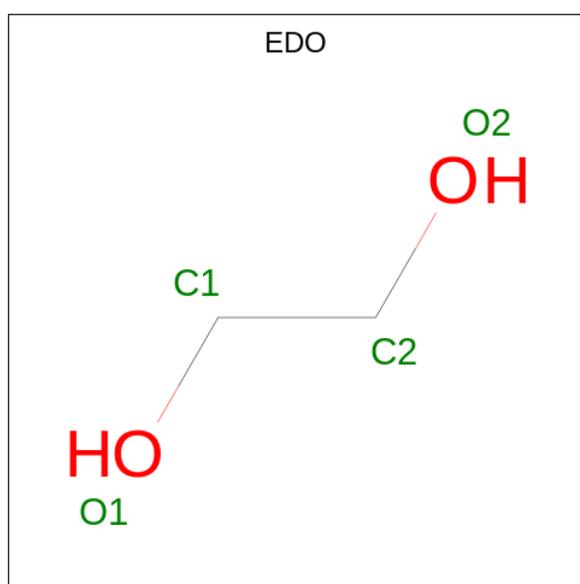
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total C H O				1	0
			10 2 6 2					
3	A	1	Total C H O				1	0
			10 2 6 2					
3	A	1	Total C H O				1	0
			10 2 6 2					
3	A	1	Total C H O				1	0
			10 2 6 2					
3	A	1	Total C H O				1	0
			10 2 6 2					
3	A	1	Total C H O				1	0
			10 2 6 2					

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 10	C 2	H 6	O 2	1	0
3	A	1	Total 10	C 2	H 6	O 2	1	0
3	A	1	Total 10	C 2	H 6	O 2	1	0
3	A	1	Total 10	C 2	H 6	O 2	1	0
3	B	1	Total 10	C 2	H 6	O 2	1	0
3	B	1	Total 10	C 2	H 6	O 2	1	0
3	B	1	Total 10	C 2	H 6	O 2	1	0
3	B	1	Total 10	C 2	H 6	O 2	1	0
3	B	1	Total 10	C 2	H 6	O 2	1	0
3	B	1	Total 10	C 2	H 6	O 2	1	0
3	B	1	Total 10	C 2	H 6	O 2	1	0
3	B	1	Total 10	C 2	H 6	O 2	1	0
3	B	1	Total 10	C 2	H 6	O 2	1	0
3	B	1	Total 10	C 2	H 6	O 2	1	0
3	C	1	Total 10	C 2	H 6	O 2	1	0
3	C	1	Total 10	C 2	H 6	O 2	1	0
3	C	1	Total 10	C 2	H 6	O 2	1	0
3	C	1	Total 10	C 2	H 6	O 2	1	0
3	C	1	Total 10	C 2	H 6	O 2	1	0
3	C	1	Total 10	C 2	H 6	O 2	1	0
3	C	1	Total 10	C 2	H 6	O 2	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total 10	C 2	H 6	O 2	1	0
3	C	1	Total 10	C 2	H 6	O 2	1	0
3	C	1	Total 10	C 2	H 6	O 2	1	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	480	Total 480	O 480	0	0
4	B	425	Total 425	O 425	0	0
4	C	509	Total 509	O 509	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: Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65
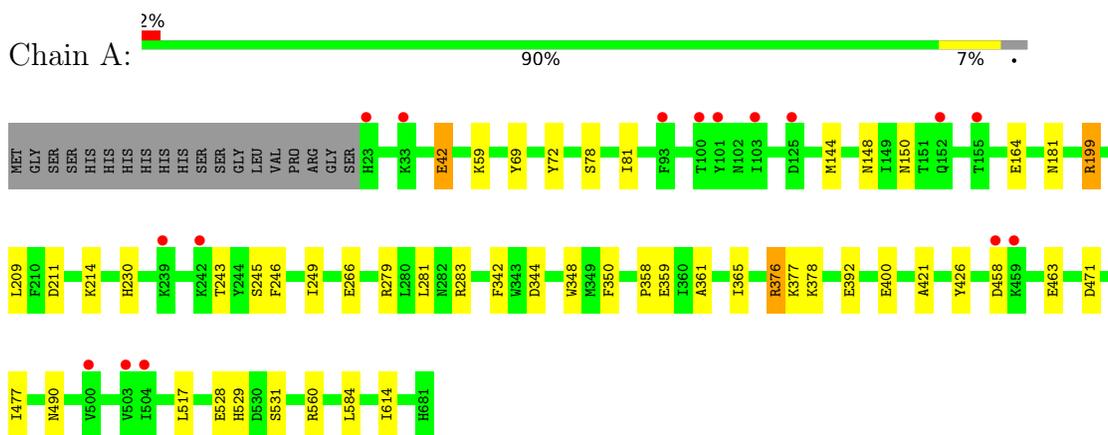
• Molecule 1: Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65

• Molecule 1: Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER H23 S30 E42 E62 Y69 R76 V77 S78 P82 N83 Y84 N85 Q99 T100 Y101 E109 N148 I149 N150 E156 E164 N174 P187 L188 L189 P196

R199 H230 A231 M232 K239 F246 S255 I258 E266 R279 R283 Q303 L315 M330 L335 D344 W348 M349 F350 E359 I360 A361 Y367 R368 D373 R376 K377 W391 E400 P441 D458 K459 Y482 N490 T499

V500 L501 G502 V503 I504 R560 Q594 P605 I614 K618 Y624 L633 K675 T676 H681
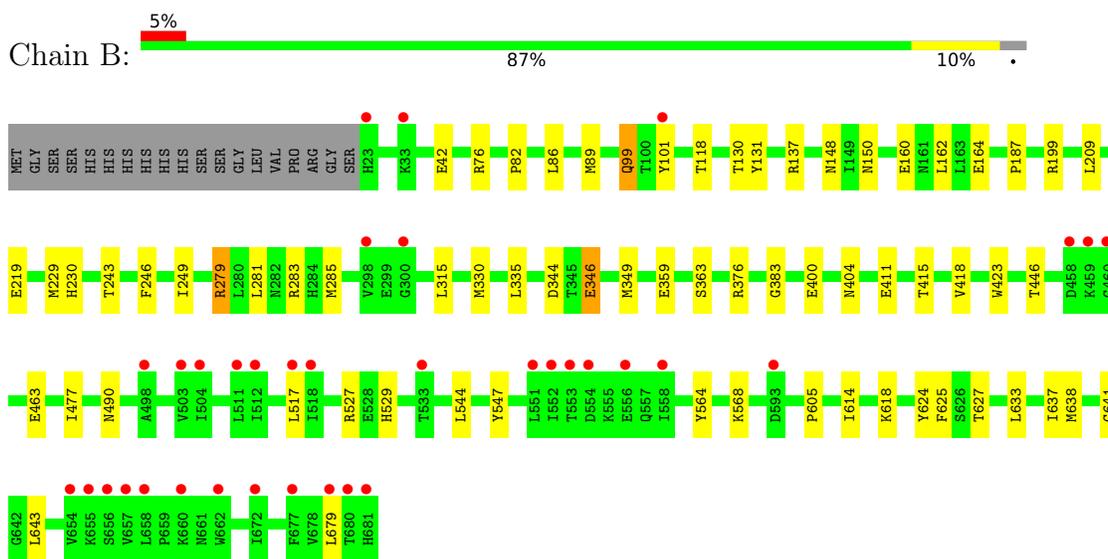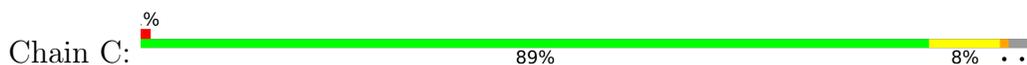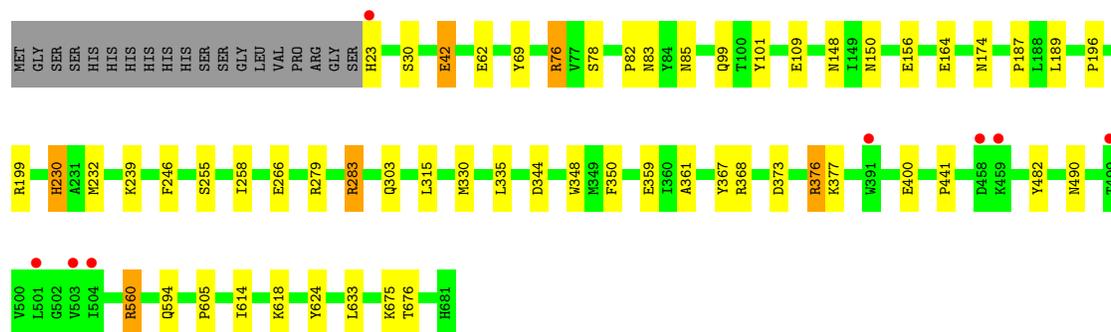
• Molecule 2: alpha-D-glucopyranose-(1-6)-beta-D-glucopyranose

Chain D:

50%　　　　　　　　　50%

BGC1 GLC2

• Molecule 2: alpha-D-glucopyranose-(1-6)-beta-D-glucopyranose

Chain E:

50%　　　　　　　　　50%

BGC1 GLC2

• Molecule 2: alpha-D-glucopyranose-(1-6)-beta-D-glucopyranose

Chain F:

50%　　　　　　　　　50%

BGC1 GLC2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	122.94Å 194.09Å 111.88Å 90.00° 116.35° 90.00°	Depositor
Resolution (Å)	44.71 – 1.56 44.67 – 1.56	Depositor EDS
% Data completeness (in resolution range)	98.3 (44.71-1.56) 98.3 (44.67-1.56)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 1.56Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.187 , 0.211 0.201 , 0.223	Depositor DCC
R_{free} test set	16344 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 39.4	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	33574	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[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: EDO, BGC, GLC

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	0.77	7/5463 (0.1%)	1.00	12/7412 (0.2%)
1	B	0.78	8/5463 (0.1%)	1.03	8/7412 (0.1%)
1	C	0.77	8/5505 (0.1%)	1.02	10/7467 (0.1%)
All	All	0.77	23/16431 (0.1%)	1.02	30/22291 (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	2
1	B	0	2
1	C	0	1
All	All	0	5

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	400	GLU	CD-OE1	10.30	1.36	1.25
1	A	164	GLU	CD-OE1	-8.81	1.16	1.25
1	C	164	GLU	CD-OE2	-8.70	1.16	1.25
1	B	164	GLU	CD-OE2	-8.32	1.16	1.25
1	A	164	GLU	CD-OE2	-8.23	1.16	1.25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	376	ARG	NE-CZ-NH2	-12.09	114.25	120.30
1	A	376	ARG	NE-CZ-NH2	-10.62	114.99	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	376	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	A	199	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	458	ASP	CB-CA-C	-7.28	95.85	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	376	ARG	Sidechain
1	A	81	ILE	Mainchain
1	B	279	ARG	Sidechain
1	B	76	ARG	Sidechain
1	C	76	ARG	Sidechain

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	5322	5233	5212	26	0
1	B	5316	5229	5212	39	0
1	C	5355	5267	5249	26	0
2	D	23	23	21	1	0
2	E	23	23	21	1	0
2	F	23	23	21	1	0
3	A	40	60	60	6	0
3	B	40	60	60	6	0
3	C	40	60	60	2	0
4	A	480	0	0	3	1
4	B	425	0	0	6	1
4	C	509	0	0	6	0
All	All	17596	15978	15916	93	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 3.

The worst 5 of 93 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:148:ASN:OD1	1:A:245[B]:SER:OG	1.86	0.91
1:A:614:ILE:HD11	3:A:707:EDO:H21	1.60	0.84
1:A:209:LEU:HD11	1:A:249:ILE:HD11	1.63	0.79
1:A:209:LEU:HD11	1:A:249:ILE:CD1	2.15	0.76
1:B:209:LEU:HD11	1:B:249:ILE:CD1	2.16	0.75

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)
4:A:1126:HOH:O	4:B:1088:HOH:O[2_555]	2.18	0.02

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	669/678 (99%)	645 (96%)	24 (4%)	0	100	100
1	B	669/678 (99%)	645 (96%)	24 (4%)	0	100	100
1	C	673/678 (99%)	654 (97%)	19 (3%)	0	100	100
All	All	2011/2034 (99%)	1944 (97%)	67 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	577/581 (99%)	572 (99%)	5 (1%)	78	61
1	B	577/581 (99%)	571 (99%)	6 (1%)	76	57
1	C	581/581 (100%)	573 (99%)	8 (1%)	67	41
All	All	1735/1743 (100%)	1716 (99%)	19 (1%)	73	53

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	196	PRO
1	C	441	PRO
1	C	490	ASN
1	C	279	ARG
1	B	279	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	286	GLN
1	B	594	GLN
1	C	681	HIS
1	C	150	ASN
1	C	158	ASN

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 ⓘ

6 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	1.51	2 (16%)	17,17,17	1.38	3 (17%)
2	GLC	D	2	2	11,11,12	0.94	0	15,15,17	1.20	1 (6%)
2	BGC	E	1	2	12,12,12	1.86	4 (33%)	17,17,17	1.62	3 (17%)
2	GLC	E	2	2	11,11,12	2.57	1 (9%)	15,15,17	1.40	1 (6%)
2	BGC	F	1	2	12,12,12	1.25	2 (16%)	17,17,17	1.70	6 (35%)
2	GLC	F	2	2	11,11,12	1.39	1 (9%)	15,15,17	1.36	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	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	F	1	2	-	0/2/22/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	GLC	C2-C3	-8.14	1.40	1.52
2	E	1	BGC	C4-C5	4.15	1.61	1.53
2	D	1	BGC	C4-C5	3.81	1.61	1.53
2	F	2	GLC	O5-C1	2.88	1.48	1.43
2	E	1	BGC	C4-C3	2.77	1.59	1.52

The worst 5 of 15 bond angle outliers are listed below:

| Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2	GLC	C1-O5-C5	4.26	117.97	112.19
2	E	2	GLC	C1-O5-C5	3.53	116.97	112.19
2	F	1	BGC	O5-C1-C2	3.37	116.30	110.28
2	E	1	BGC	O3-C3-C4	3.13	117.58	110.35
2	F	1	BGC	O4-C4-C5	-2.93	102.02	109.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	BGC	1	0
2	E	2	GLC	1	0
2	F	2	GLC	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.

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings
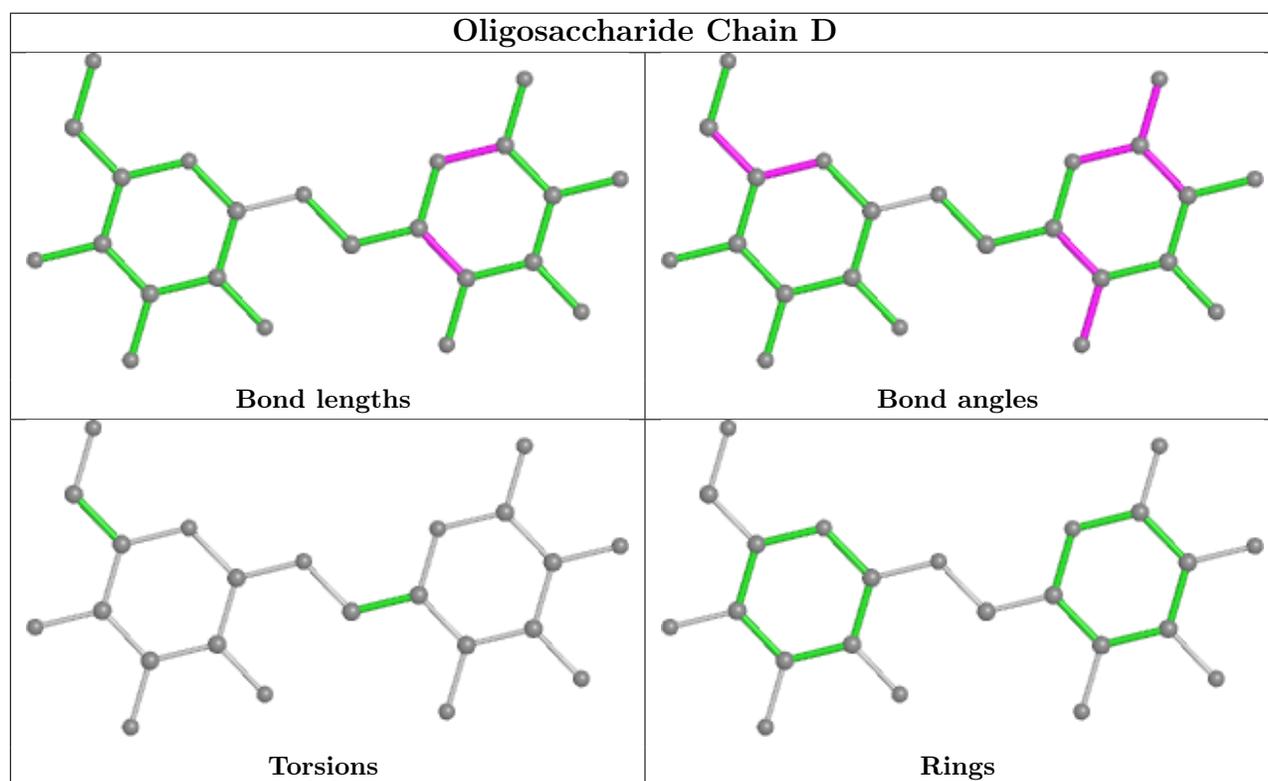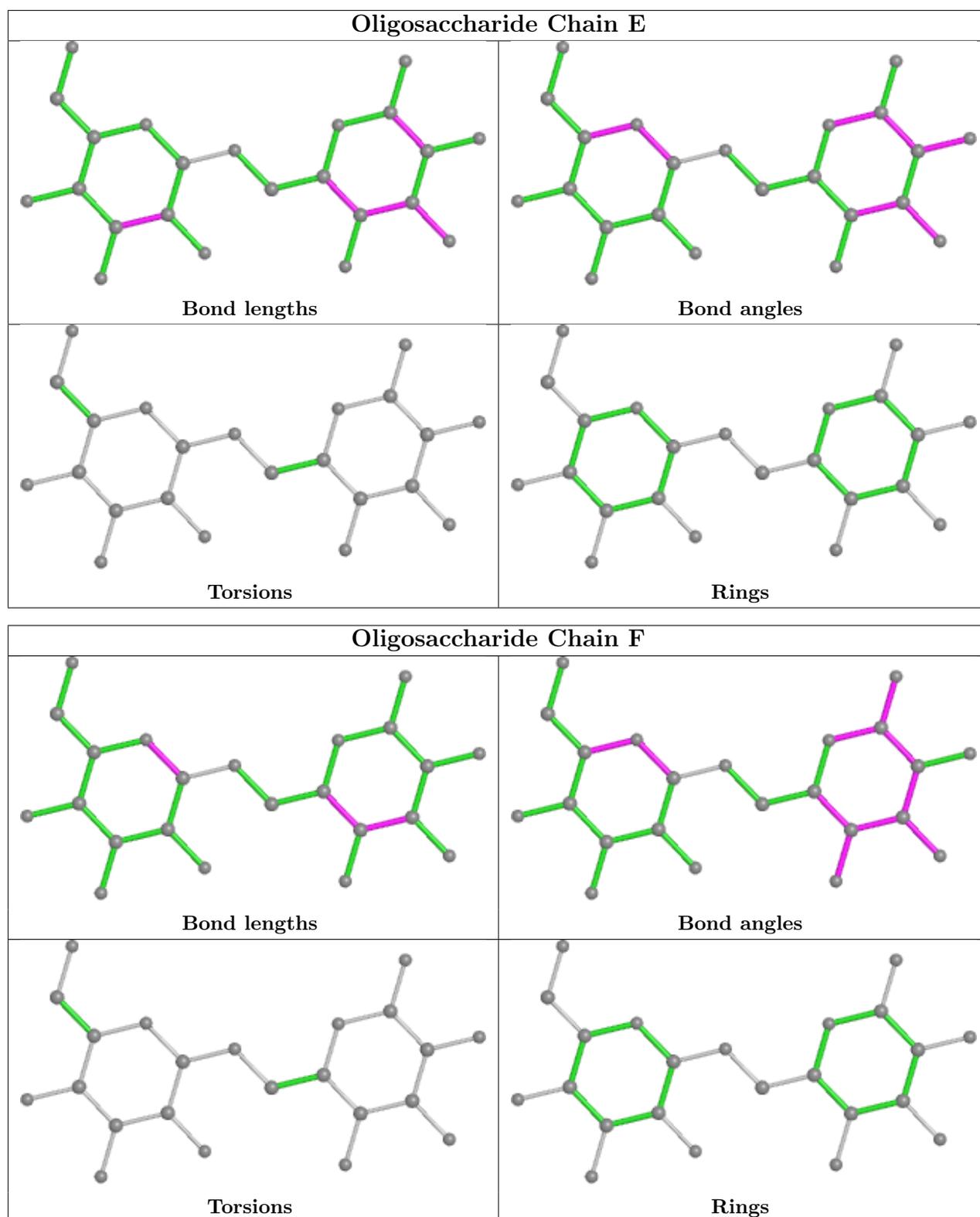
5.6 Ligand geometry ⓘ

30 ligands 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	$\#|Z| > 2$
3	EDO	A	703	-	3,3,3	0.41	0	2,2,2	0.50	0
3	EDO	B	711	-	3,3,3	0.33	0	2,2,2	0.79	0
3	EDO	B	709	-	3,3,3	0.52	0	2,2,2	0.34	0
3	EDO	B	705	-	3,3,3	0.65	0	2,2,2	0.55	0
3	EDO	B	710	-	3,3,3	0.33	0	2,2,2	0.73	0
3	EDO	A	706	-	3,3,3	0.86	0	2,2,2	0.27	0
3	EDO	C	706	-	3,3,3	0.42	0	2,2,2	0.40	0
3	EDO	C	709	-	3,3,3	0.18	0	2,2,2	0.84	0
3	EDO	A	712	-	3,3,3	0.93	0	2,2,2	1.01	0
3	EDO	C	703	-	3,3,3	0.47	0	2,2,2	0.55	0
3	EDO	A	709	-	3,3,3	0.35	0	2,2,2	0.40	0
3	EDO	C	707	-	3,3,3	0.36	0	2,2,2	0.14	0
3	EDO	C	708	-	3,3,3	0.19	0	2,2,2	0.24	0
3	EDO	B	706	-	3,3,3	1.12	0	2,2,2	0.61	0
3	EDO	A	710	-	3,3,3	0.32	0	2,2,2	0.45	0
3	EDO	C	704	-	3,3,3	0.54	0	2,2,2	0.31	0
3	EDO	C	702	-	3,3,3	0.37	0	2,2,2	0.32	0
3	EDO	A	707	-	3,3,3	0.94	0	2,2,2	1.08	0
3	EDO	C	701	-	3,3,3	0.47	0	2,2,2	0.31	0
3	EDO	B	707	-	3,3,3	0.85	0	2,2,2	0.49	0
3	EDO	B	704	-	3,3,3	0.25	0	2,2,2	0.55	0
3	EDO	B	703	-	3,3,3	0.50	0	2,2,2	0.85	0
3	EDO	A	708	-	3,3,3	0.36	0	2,2,2	0.23	0
3	EDO	B	712	-	3,3,3	0.30	0	2,2,2	1.06	0
3	EDO	B	708	-	3,3,3	1.00	0	2,2,2	0.50	0
3	EDO	A	705	-	3,3,3	0.54	0	2,2,2	0.41	0
3	EDO	A	711	-	3,3,3	0.12	0	2,2,2	0.77	0
3	EDO	A	704	-	3,3,3	0.55	0	2,2,2	0.63	0
3	EDO	C	710	-	3,3,3	0.17	0	2,2,2	0.29	0
3	EDO	C	705	-	3,3,3	0.84	0	2,2,2	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	703	-	-	0/1/1/1	-
3	EDO	B	711	-	-	1/1/1/1	-
3	EDO	B	709	-	-	1/1/1/1	-
3	EDO	B	705	-	-	1/1/1/1	-
3	EDO	B	710	-	-	0/1/1/1	-
3	EDO	A	706	-	-	1/1/1/1	-
3	EDO	C	706	-	-	1/1/1/1	-
3	EDO	C	709	-	-	1/1/1/1	-
3	EDO	A	712	-	-	1/1/1/1	-
3	EDO	C	703	-	-	0/1/1/1	-
3	EDO	A	709	-	-	1/1/1/1	-
3	EDO	C	707	-	-	0/1/1/1	-
3	EDO	C	708	-	-	0/1/1/1	-
3	EDO	B	706	-	-	1/1/1/1	-
3	EDO	A	710	-	-	0/1/1/1	-
3	EDO	C	704	-	-	0/1/1/1	-
3	EDO	C	702	-	-	0/1/1/1	-
3	EDO	A	707	-	-	0/1/1/1	-
3	EDO	C	701	-	-	0/1/1/1	-
3	EDO	B	707	-	-	0/1/1/1	-
3	EDO	B	704	-	-	0/1/1/1	-
3	EDO	B	703	-	-	0/1/1/1	-
3	EDO	A	708	-	-	0/1/1/1	-
3	EDO	B	712	-	-	1/1/1/1	-
3	EDO	B	708	-	-	0/1/1/1	-
3	EDO	A	705	-	-	1/1/1/1	-
3	EDO	A	711	-	-	1/1/1/1	-
3	EDO	A	704	-	-	0/1/1/1	-
3	EDO	C	710	-	-	1/1/1/1	-
3	EDO	C	705	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	711	EDO	O1-C1-C2-O2
3	A	705	EDO	O1-C1-C2-O2
3	A	709	EDO	O1-C1-C2-O2
3	B	705	EDO	O1-C1-C2-O2
3	B	711	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	705	EDO	2	0
3	A	706	EDO	2	0
3	C	704	EDO	1	0
3	A	707	EDO	3	0
3	B	707	EDO	1	0
3	B	708	EDO	3	0
3	A	705	EDO	1	0
3	C	705	EDO	1	0

5.7 Other polymers ⓘ

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, 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	659/678 (97%)	-0.09	16 (2%)	59	65	18, 26, 46, 71	0
1	B	659/678 (97%)	0.16	35 (5%)	26	31	17, 29, 50, 70	0
1	C	659/678 (97%)	-0.18	8 (1%)	79	83	17, 25, 41, 57	0
All	All	1977/2034 (97%)	-0.04	59 (2%)	50	58	17, 26, 46, 71	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	504	ILE	6.7
1	A	101	TYR	6.6
1	B	517	LEU	5.3
1	B	511	LEU	4.6
1	B	552	ILE	4.4

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	F	1	12/12	0.72	0.17	34,43,45,48	4
2	BGC	D	1	12/12	0.86	0.12	26,34,43,43	4
2	BGC	E	1	12/12	0.89	0.09	27,33,43,43	4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	GLC	D	2	11/12	0.96	0.09	18,20,43,43	4
2	GLC	F	2	11/12	0.96	0.08	21,24,43,43	4
2	GLC	E	2	11/12	0.97	0.11	17,20,43,43	4

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)
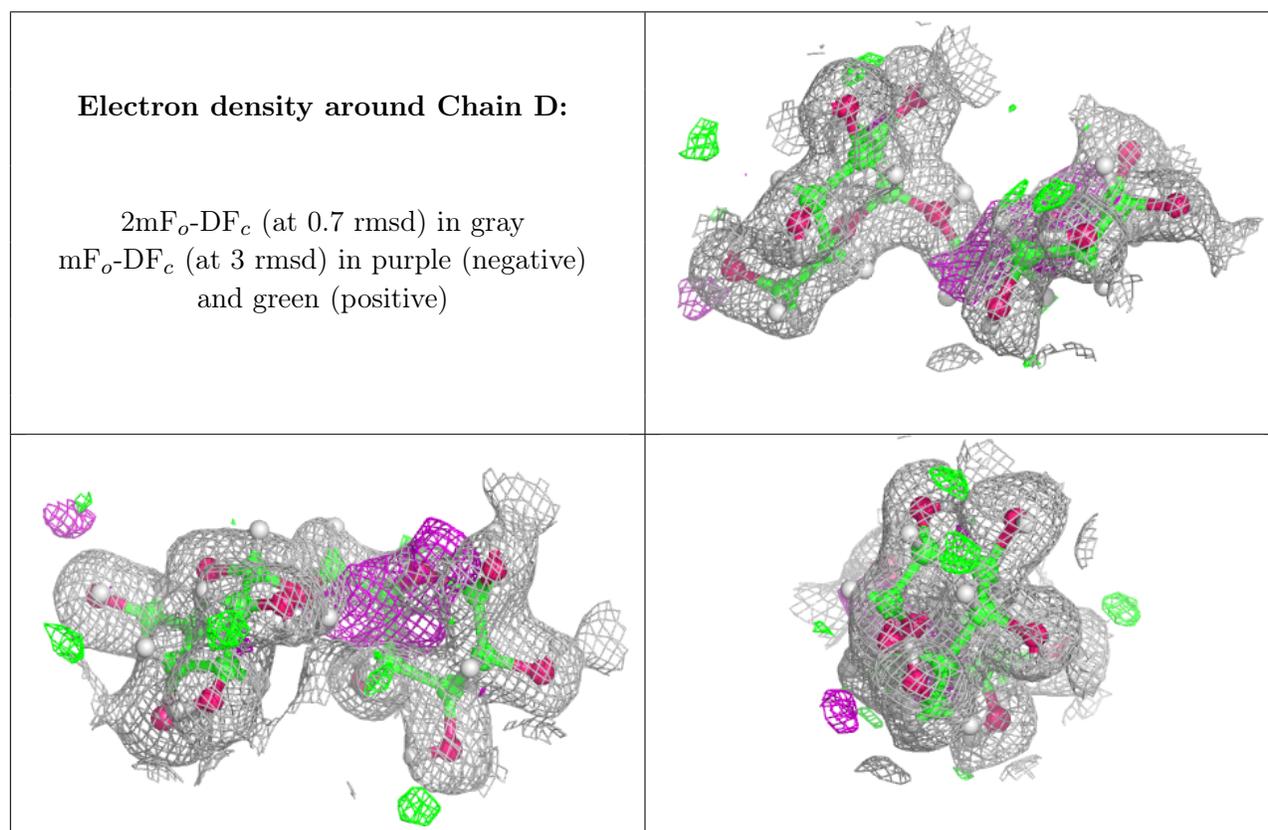
Electron density around Chain E:

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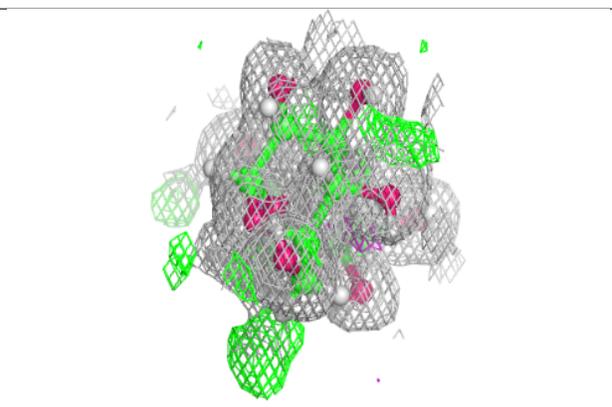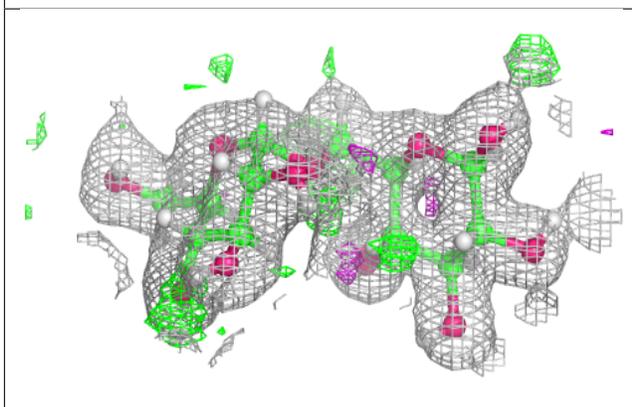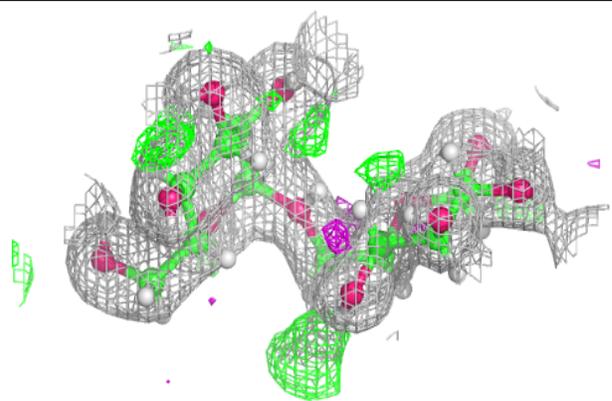
Electron density around Chain F:

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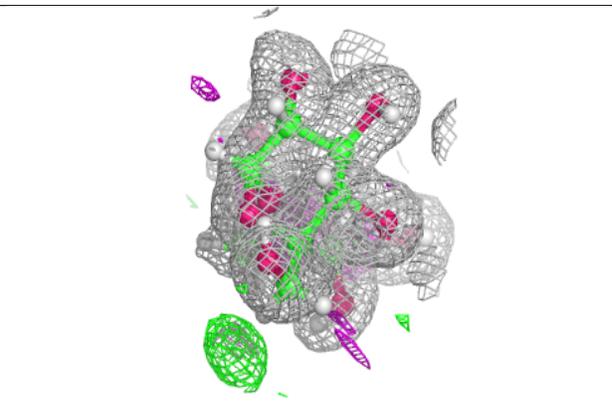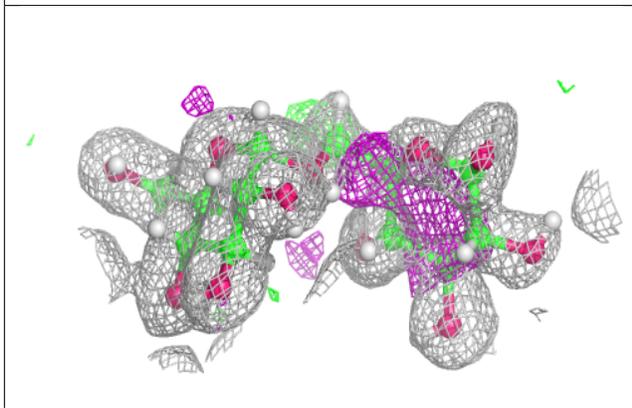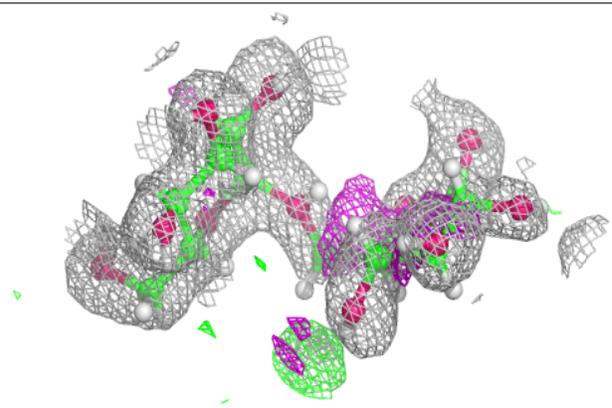
6.4 Ligands ⓘ

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
3	EDO	A	712	4/4	0.68	0.28	43,52,52,53	1
3	EDO	C	708	4/4	0.75	0.15	43,51,54,55	1
3	EDO	B	706	4/4	0.76	0.21	43,45,46,47	1
3	EDO	B	712	4/4	0.78	0.18	43,52,54,54	1
3	EDO	B	710	4/4	0.85	0.23	37,43,47,50	1
3	EDO	B	708	4/4	0.86	0.17	31,36,38,43	1
3	EDO	B	705	4/4	0.88	0.09	33,34,43,46	1
3	EDO	A	711	4/4	0.88	0.16	40,41,46,51	1
3	EDO	A	706	4/4	0.89	0.14	35,39,43,44	1
3	EDO	B	707	4/4	0.89	0.07	33,34,35,43	1
3	EDO	C	710	4/4	0.90	0.16	43,48,53,59	1
3	EDO	C	709	4/4	0.91	0.10	43,49,56,59	1
3	EDO	A	708	4/4	0.91	0.12	34,39,41,43	1
3	EDO	C	704	4/4	0.92	0.10	34,36,42,43	1
3	EDO	C	705	4/4	0.93	0.10	25,31,35,43	1
3	EDO	A	705	4/4	0.94	0.09	29,31,43,45	1
3	EDO	C	706	4/4	0.94	0.11	33,37,38,43	1
3	EDO	C	707	4/4	0.94	0.17	37,39,41,43	1
3	EDO	A	707	4/4	0.95	0.11	24,31,37,43	1
3	EDO	A	709	4/4	0.96	0.17	29,42,43,44	1
3	EDO	B	703	4/4	0.97	0.11	24,26,31,43	1
3	EDO	B	704	4/4	0.97	0.10	25,26,27,43	1
3	EDO	B	709	4/4	0.97	0.07	36,37,38,43	1
3	EDO	A	703	4/4	0.97	0.08	19,20,22,43	1
3	EDO	B	711	4/4	0.97	0.08	33,38,43,43	1
3	EDO	A	710	4/4	0.97	0.16	34,39,42,43	1
3	EDO	C	701	4/4	0.97	0.08	20,23,25,43	1
3	EDO	C	702	4/4	0.98	0.11	21,26,28,43	1
3	EDO	C	703	4/4	0.98	0.04	29,37,40,43	1
3	EDO	A	704	4/4	0.98	0.08	20,23,27,43	1

6.5 Other polymers ⓘ

There are no such residues in this entry.