



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 06:06 PM UTC

PDB ID : 7PRB / pdb\_00007prb  
Title : Crystal structure of Burkholderia pseudomallei heparanase in complex with covalent inhibitor GR109  
Authors : Wu, L.; Armstrong, Z.; Davies, G.J.  
Deposited on : 2021-09-21  
Resolution : 1.31 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

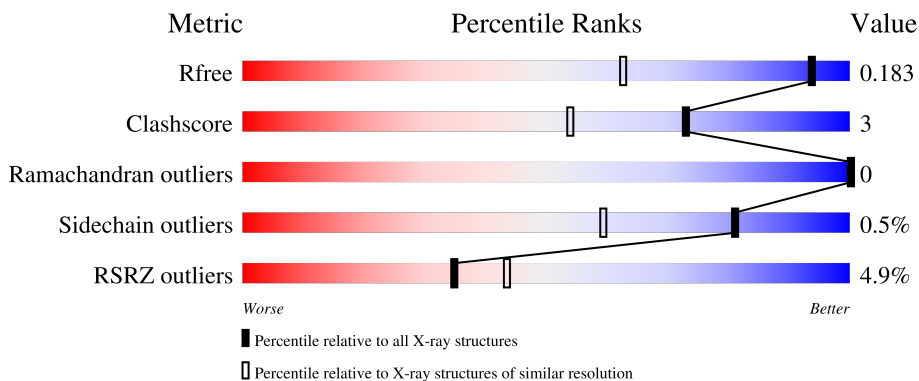
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.31 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))
$R_{free}$	180053	2531 (1.34-1.30)
Clashscore	190562	2585 (1.34-1.30)
Ramachandran outliers	187476	2528 (1.34-1.30)
Sidechain outliers	187428	2528 (1.34-1.30)
RSRZ outliers	180081	2528 (1.34-1.30)

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	438	 2% 92% 7%
1	B	438	 8% 96% .
2	C	2	 100%
2	D	2	 100%

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
3	EDO	A	502	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13988 atoms, of which 6411 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.

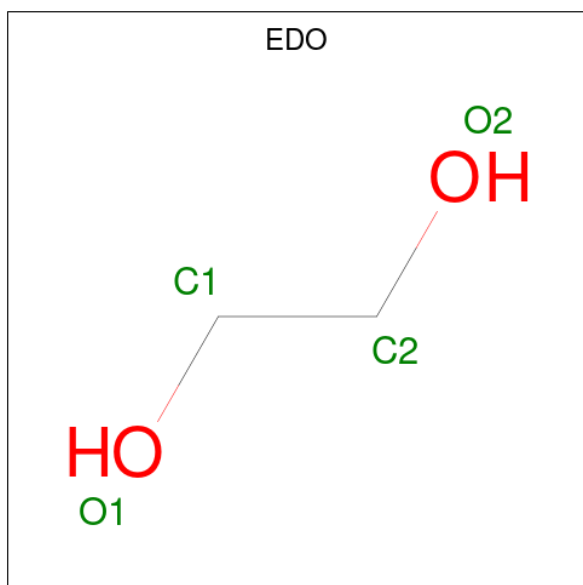
- Molecule 1 is a protein called Glyco\_hydro\_44 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	437	Total 6480	C 2054	H 3201	N 584	O 632	S 9	92	17	0
1	B	438	Total 6291	C 2001	H 3105	N 560	O 615	S 10	90	5	0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-(2R,3S,5R,6R)-2,3,4,5,6-pentakis(oxidanyl)cyclohexane-1-carboxylic acid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	C	2	Total 104	C 30	H 42	N 2	O 28	S 2	10	2	0
2	D	2	Total 52	C 15	H 21	N 1	O 14	S 1	5	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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	B	1	Total	C	H	O	1	0
			10	2	6	2		
3	B	1	Total	C	H	O	1	0
			10	2	6	2		

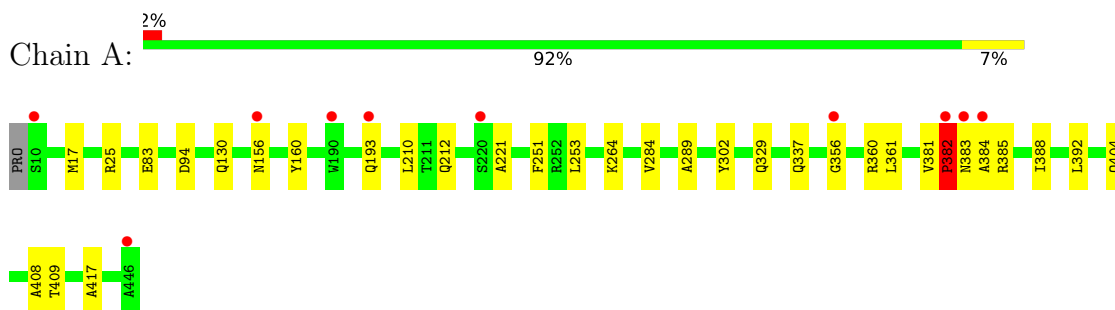
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	574	Total	O	0	0
			574	574		
4	B	417	Total	O	0	0
			417	417		

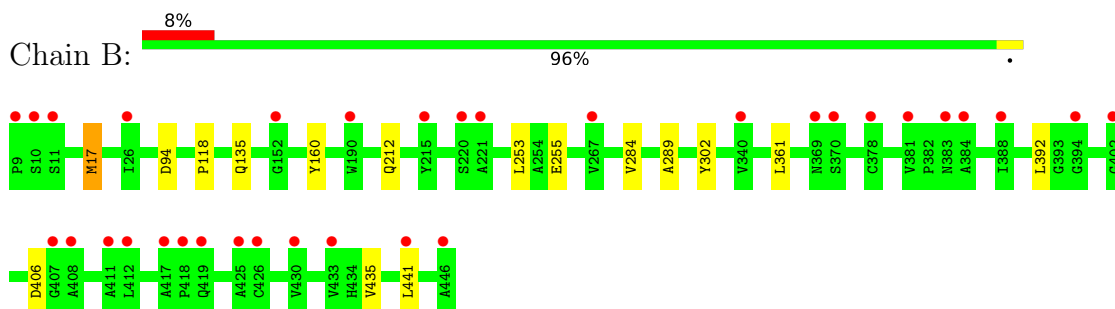
### 3 Residue-property plots [i](#)

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.

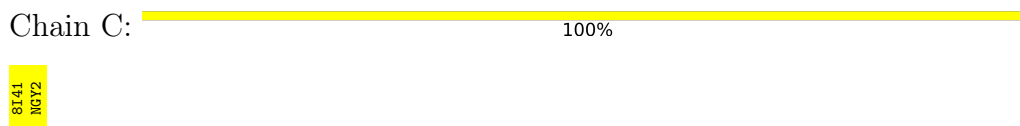
- Molecule 1: Glyco\_hydro\_44 domain-containing protein



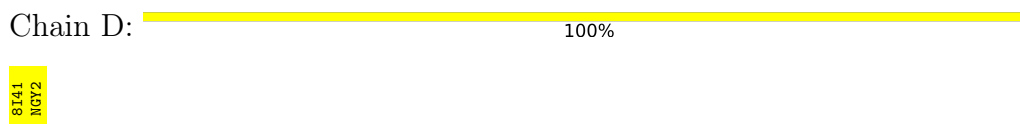
- Molecule 1: Glyco\_hydro\_44 domain-containing protein



- Molecule 2: 2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-(2R,3S,5R,6R)-2,3,4,5,6-pentakis(oxidanyl)cyclohexane-1-carboxylic acid



- Molecule 2: 2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-(2R,3S,5R,6R)-2,3,4,5,6-pentakis(oxidanyl)cyclohexane-1-carboxylic acid



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.21Å 101.07Å 113.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.06 – 1.31 66.06 – 1.31	Depositor EDS
% Data completeness (in resolution range)	98.4 (66.06-1.31) 98.3 (66.06-1.31)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 1.31Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.166 , 0.185 0.164 , 0.183	Depositor DCC
$R_{free}$ test set	11043 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.4	Xtrriage
Anisotropy	0.576	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 38.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	13988	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: NGY, 8I4, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.10	0/3350	1.17	10/4573 (0.2%)
1	B	1.10	1/3257 (0.0%)	1.16	1/4449 (0.0%)
All	All	1.10	1/6607 (0.0%)	1.17	11/9022 (0.1%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	GLU	CD-OE2	6.09	1.36	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382[A]	PRO	CA-C-N	-6.25	109.87	122.55
1	A	382[A]	PRO	C-N-CA	-6.25	109.87	122.55
1	A	382[B]	PRO	CA-C-N	-6.25	109.87	122.55
1	A	382[B]	PRO	C-N-CA	-6.25	109.87	122.55
1	A	382[A]	PRO	CA-C-O	-5.62	115.22	121.23
1	A	382[B]	PRO	CA-C-O	-5.62	115.22	121.23
1	A	160	TYR	O-C-N	-5.43	115.65	120.48
1	A	25	ARG	CG-CD-NE	-5.42	100.07	112.00
1	A	94	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	160	TYR	O-C-N	-5.32	115.50	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	ARG	N-CA-C	-5.23	106.75	113.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	382[B]	PRO	Mainchain

## 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	3279	3201	3178	30	0
1	B	3186	3105	3092	10	0
2	C	62	42	16	0	0
2	D	31	21	8	0	0
3	A	20	30	29	5	0
3	B	8	12	12	0	0
4	A	574	0	0	17	1
4	B	417	0	0	3	1
All	All	7577	6411	6335	41	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.

All (41) 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:130[B]:GLN:HG3	4:A:619:HOH:O	1.61	1.00
1:A:408:ALA:HB1	3:A:502:EDO:H21	1.49	0.94
1:B:94:ASP:OD1	4:B:602:HOH:O	1.90	0.90
3:A:502:EDO:H11	4:A:736:HOH:O	1.71	0.90
1:A:337[B]:GLN:NE2	4:A:601:HOH:O	2.12	0.82
1:A:408:ALA:CB	3:A:502:EDO:H21	2.13	0.79
1:A:156:ASN:HB3	4:A:604:HOH:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360[B]:ARG:NH2	4:A:603:HOH:O	2.23	0.71
1:B:435:VAL:HG22	1:B:441:LEU:HD12	1.75	0.69
1:A:156:ASN:HB2	4:A:958:HOH:O	1.93	0.67
1:A:409:THR:HG22	4:A:649:HOH:O	1.98	0.63
1:A:156:ASN:ND2	4:A:604:HOH:O	2.27	0.62
1:A:329:GLN:O	1:A:360[A]:ARG:HD3	2.01	0.60
1:A:337[A]:GLN:NE2	4:A:605:HOH:O	2.35	0.59
1:A:17[B]:MET:HE1	1:A:361:LEU:HD22	1.84	0.58
1:A:356:GLY:HA3	4:A:603:HOH:O	2.03	0.58
1:B:17[B]:MET:HE1	1:B:361:LEU:HD22	1.89	0.54
3:A:505:EDO:H12	4:A:696:HOH:O	2.08	0.52
1:A:417:ALA:H	3:A:502:EDO:C2	2.23	0.51
1:A:83:GLU:OE1	4:A:602:HOH:O	2.19	0.49
1:B:284:VAL:HG12	1:B:289:ALA:HB3	1.95	0.48
1:B:392:LEU:C	1:B:392:LEU:HD23	2.39	0.48
1:B:212:GLN:O	1:B:253:LEU:HA	2.13	0.47
1:A:193[A]:GLN:NE2	4:A:608:HOH:O	2.39	0.47
1:A:356:GLY:CA	4:A:603:HOH:O	2.63	0.46
1:A:392:LEU:C	1:A:392:LEU:HD23	2.42	0.45
1:A:382[A]:PRO:O	1:A:383:ASN:C	2.59	0.45
1:A:221:ALA:HB3	1:A:264:LYS:HG2	1.99	0.45
1:A:382[A]:PRO:HG3	1:B:135:GLN:HG2	1.98	0.45
1:B:435:VAL:HG22	1:B:441:LEU:CD1	2.44	0.44
1:A:284:VAL:HG12	1:A:289:ALA:HB3	2.00	0.44
1:A:409:THR:CG2	4:A:649:HOH:O	2.63	0.43
1:A:156:ASN:CB	4:A:958:HOH:O	2.60	0.43
1:A:381[A]:VAL:HG11	1:A:384:ALA:HB2	2.02	0.42
1:B:118:PRO:HB2	4:B:946:HOH:O	2.18	0.42
1:A:404:GLN:HG2	1:A:409:THR:HG22	2.01	0.42
1:A:210:LEU:O	1:A:251:PHE:HA	2.19	0.42
1:A:212:GLN:O	1:A:253:LEU:HA	2.20	0.42
1:A:388[A]:ILE:HD12	4:A:805:HOH:O	2.21	0.41
1:B:406:ASP:HA	4:B:601:HOH:O	2.20	0.41
1:A:17[B]:MET:HE1	1:A:361:LEU:HD13	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1129:HOH:O	4:B:934:HOH:O[3_544]	2.12	0.08

## 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	452/438 (103%)	444 (98%)	8 (2%)	0	100	100
1	B	441/438 (101%)	433 (98%)	8 (2%)	0	100	100
All	All	893/876 (102%)	877 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	325/310 (105%)	324 (100%)	1 (0%)	86	67
1	B	315/310 (102%)	312 (99%)	3 (1%)	68	36
All	All	640/620 (103%)	636 (99%)	4 (1%)	81	54

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	TYR
1	B	17[A]	MET
1	B	17[B]	MET
1	B	302	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	ASN
1	A	428	ASN
1	B	419	GLN
1	B	428	ASN

### 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](#)

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	8I4	C	1[A]	1,2	13,13,14	1.26	1 (7%)	18,19,21	1.30	3 (16%)
2	8I4	C	1[B]	1,2	13,13,14	1.18	2 (15%)	18,19,21	1.92	5 (27%)
2	NGY	C	2[A]	2	18,18,19	0.95	0	23,26,28	1.60	6 (26%)
2	NGY	C	2[B]	2	18,18,19	0.85	1 (5%)	23,26,28	1.58	7 (30%)
2	8I4	D	1	1,2	13,13,14	2.31	3 (23%)	18,19,21	2.51	4 (22%)
2	NGY	D	2	2	18,18,19	1.01	1 (5%)	23,26,28	1.61	5 (21%)

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	8I4	C	1[A]	1,2	-	2/4/24/28	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	8I4	C	1[B]	1,2	-	0/4/24/28	0/1/1/1
2	NGY	C	2[A]	2	-	0/10/27/30	0/1/1/1
2	NGY	C	2[B]	2	-	1/10/27/30	0/1/1/1
2	8I4	D	1	1,2	-	0/4/24/28	0/1/1/1
2	NGY	D	2	2	-	0/10/27/30	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	8I4	C1-C2	-6.16	1.41	1.52
2	D	1	8I4	O6A-C6	2.75	1.30	1.22
2	C	1[A]	8I4	C1-C7	-2.74	1.47	1.52
2	C	1[B]	8I4	C1-C7	-2.60	1.47	1.52
2	D	1	8I4	C2-C3	2.56	1.56	1.52
2	C	1[B]	8I4	C1-C2	-2.27	1.48	1.52
2	D	2	NGY	O3-C3	2.16	1.48	1.43
2	C	2[B]	NGY	O6-S	-2.14	1.51	1.56

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	8I4	C1-C2-C3	-6.68	101.03	110.67
2	D	1	8I4	C7-C1-C2	5.38	117.74	111.50
2	D	1	8I4	C1-C7-C5	-4.32	104.58	111.56
2	C	2[A]	NGY	C2-N2-C7	3.82	128.02	122.90
2	D	2	NGY	O6-C6-C5	-3.80	100.79	107.57
2	C	1[B]	8I4	O7-C7-C5	-3.40	102.62	110.02
2	C	2[B]	NGY	C2-N2-C7	-3.32	118.44	122.90
2	C	1[B]	8I4	C1-C7-C5	-3.32	106.19	111.56
2	D	2	NGY	C1-O5-C5	3.26	116.55	112.19
2	C	1[B]	8I4	C1-C2-C3	-3.08	106.22	110.67
2	C	2[B]	NGY	C1-O5-C5	2.98	116.18	112.19
2	C	2[B]	NGY	C3-C4-C5	-2.79	105.18	110.23
2	C	2[B]	NGY	O4-C4-C5	2.76	116.11	109.32
2	C	2[A]	NGY	O7-C7-C8	-2.73	117.20	122.05
2	C	2[A]	NGY	O6-S-O7A	-2.63	98.90	106.92
2	C	1[B]	8I4	O4-C4-C5	-2.62	103.87	109.80
2	D	2	NGY	O9-S-O6	-2.55	100.50	106.37
2	C	1[B]	8I4	O2-C2-C1	2.49	116.04	109.86
2	C	1[A]	8I4	C1-C7-C5	-2.41	107.66	111.56
2	C	2[A]	NGY	C4-C3-C2	2.39	114.53	111.02
2	D	2	NGY	O9-S-O7A	2.38	116.87	108.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2[A]	NGY	O7-C7-N2	2.32	126.08	121.98
2	C	2[A]	NGY	O6-C6-C5	-2.28	103.51	107.57
2	D	2	NGY	O3-C3-C2	-2.23	104.78	109.40
2	C	2[B]	NGY	O6-C6-C5	-2.21	103.63	107.57
2	C	2[B]	NGY	C4-C3-C2	-2.20	107.80	111.02
2	C	1[A]	8I4	O2-C2-C1	2.20	115.32	109.86
2	C	2[B]	NGY	O9-S-O8	2.16	116.12	108.56
2	D	1	8I4	O2-C2-C1	2.14	115.19	109.86
2	C	1[A]	8I4	C7-C1-C2	2.11	113.94	111.50

There are no chirality outliers.

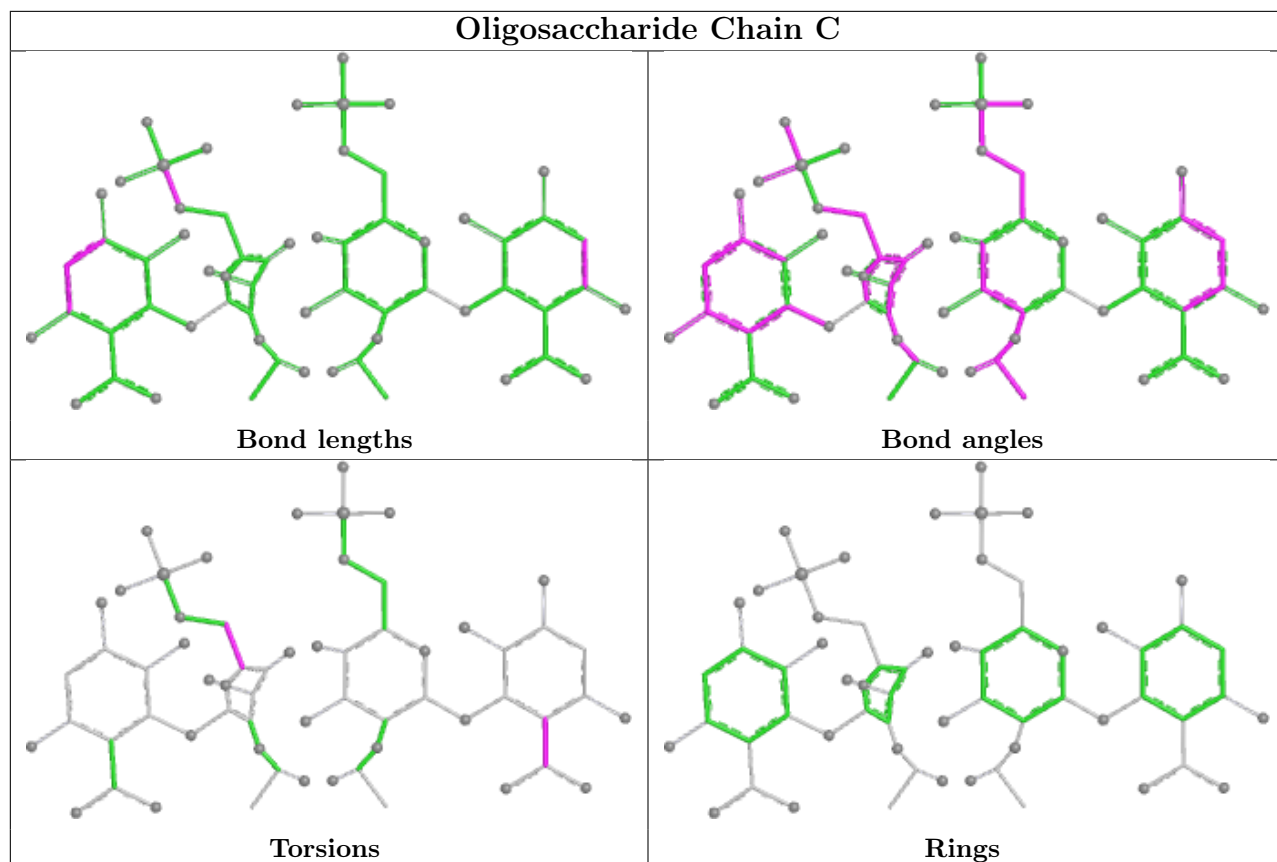
All (3) torsion outliers are listed below:

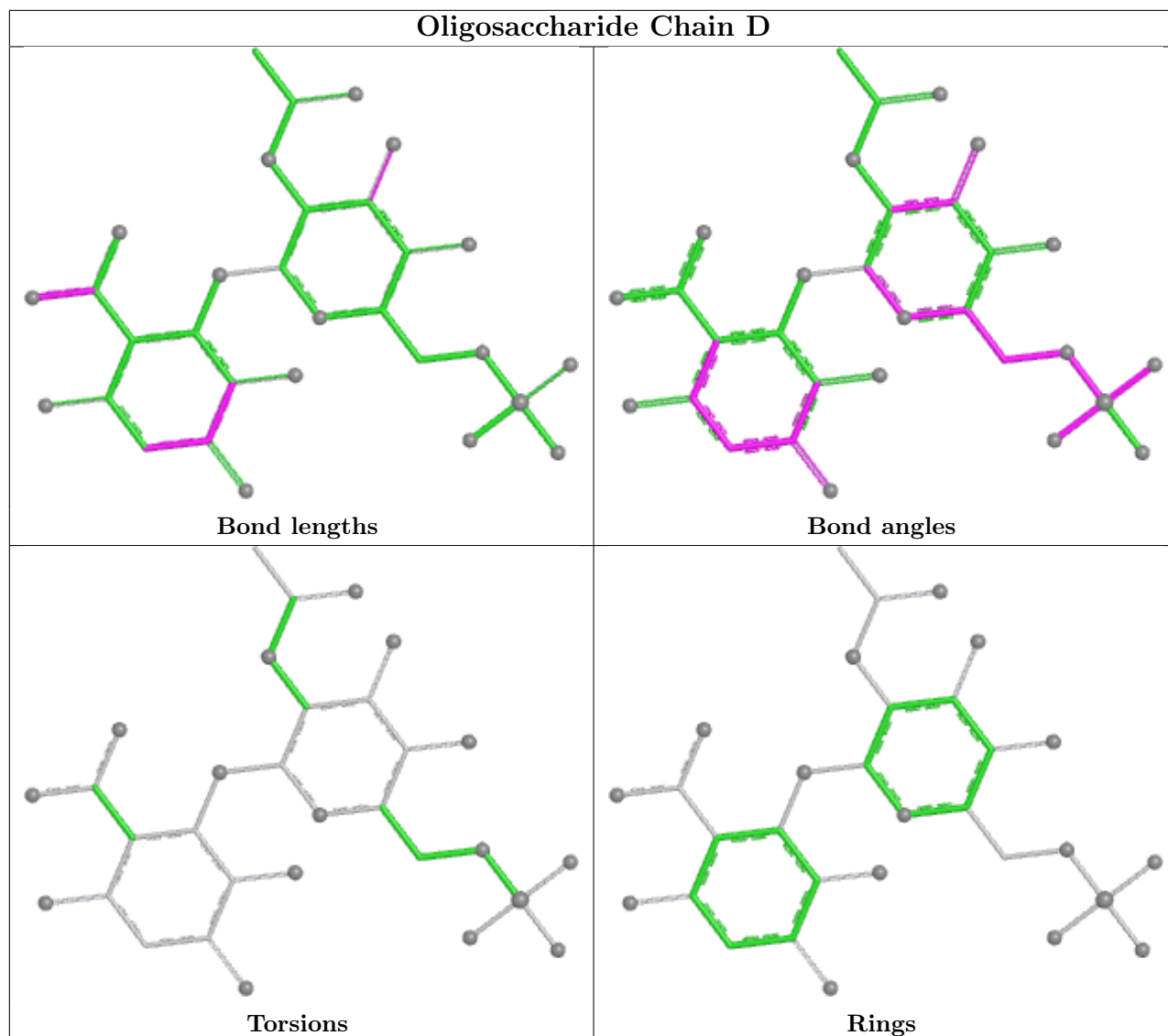
Mol	Chain	Res	Type	Atoms
2	C	2[B]	NGY	O5-C5-C6-O6
2	C	1[A]	8I4	C4-C5-C6-O6B
2	C	1[A]	8I4	C4-C5-C6-O6A

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

7 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	502	-	3,3,3	0.68	0	2,2,2	0.25	0
3	EDO	A	505	-	3,3,3	0.91	0	2,2,2	1.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	A	501	-	3,3,3	0.12	0	2,2,2	0.32	0
3	EDO	B	501	-	3,3,3	0.53	0	2,2,2	0.56	0
3	EDO	A	503	-	3,3,3	0.62	0	2,2,2	0.45	0
3	EDO	A	504	-	3,3,3	0.23	0	2,2,2	0.42	0
3	EDO	B	502	-	3,3,3	0.38	0	2,2,2	0.40	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	502	-	-	0/1/1/1	-
3	EDO	A	505	-	-	0/1/1/1	-
3	EDO	A	501	-	-	0/1/1/1	-
3	EDO	B	501	-	-	0/1/1/1	-
3	EDO	A	503	-	-	0/1/1/1	-
3	EDO	A	504	-	-	1/1/1/1	-
3	EDO	B	502	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	EDO	4	0
3	A	505	EDO	1	0

## 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	437/438 (99%)	-0.05	10 (2%) 61 68	8, 18, 30, 62	17 (3%)
1	B	438/438 (100%)	0.60	33 (7%) 20 25	10, 25, 41, 84	5 (1%)
All	All	875/876 (99%)	0.28	43 (4%) 35 43	8, 21, 38, 84	22 (2%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	382[A]	PRO	8.1
1	B	9	PRO	4.3
1	A	384	ALA	3.5
1	B	10	SER	3.5
1	B	221	ALA	3.5
1	B	446	ALA	3.1
1	B	433	VAL	3.1
1	A	220	SER	3.0
1	A	446	ALA	3.0
1	B	417	ALA	2.9
1	B	425	ALA	2.8
1	B	426	CYS	2.7
1	B	394	GLY	2.7
1	B	11	SER	2.7
1	B	384	ALA	2.6
1	B	215	TYR	2.6
1	B	441	LEU	2.6
1	B	383	ASN	2.6
1	B	267	VAL	2.6
1	A	156	ASN	2.5
1	A	10	SER	2.5
1	B	408	ALA	2.5
1	A	190	TRP	2.5
1	B	152	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	402	GLY	2.4
1	B	378	CYS	2.4
1	B	412	LEU	2.4
1	A	383	ASN	2.4
1	B	419	GLN	2.3
1	B	411	ALA	2.3
1	B	430	VAL	2.3
1	B	220	SER	2.2
1	B	418	PRO	2.2
1	B	369	ASN	2.2
1	B	381	VAL	2.2
1	A	193[A]	GLN	2.1
1	A	356	GLY	2.1
1	B	26	ILE	2.1
1	B	388	ILE	2.1
1	B	340	VAL	2.1
1	B	370	SER	2.1
1	B	190	TRP	2.0
1	B	407	GLY	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](#)

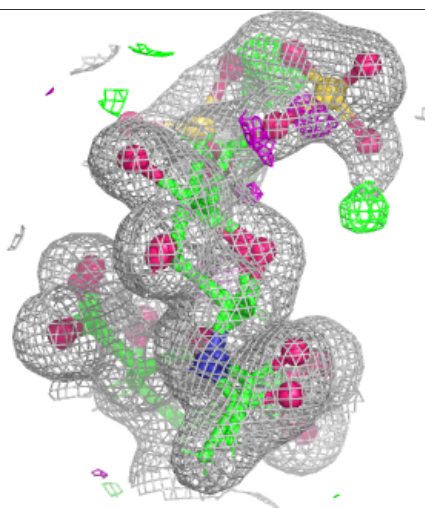
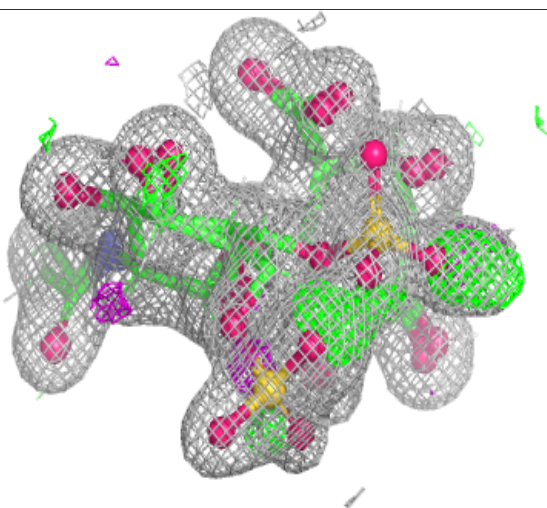
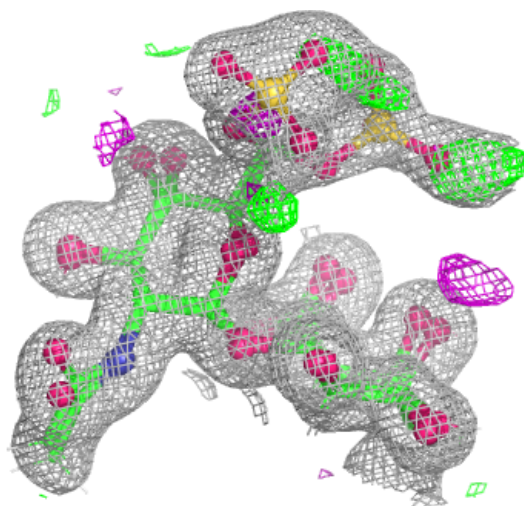
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

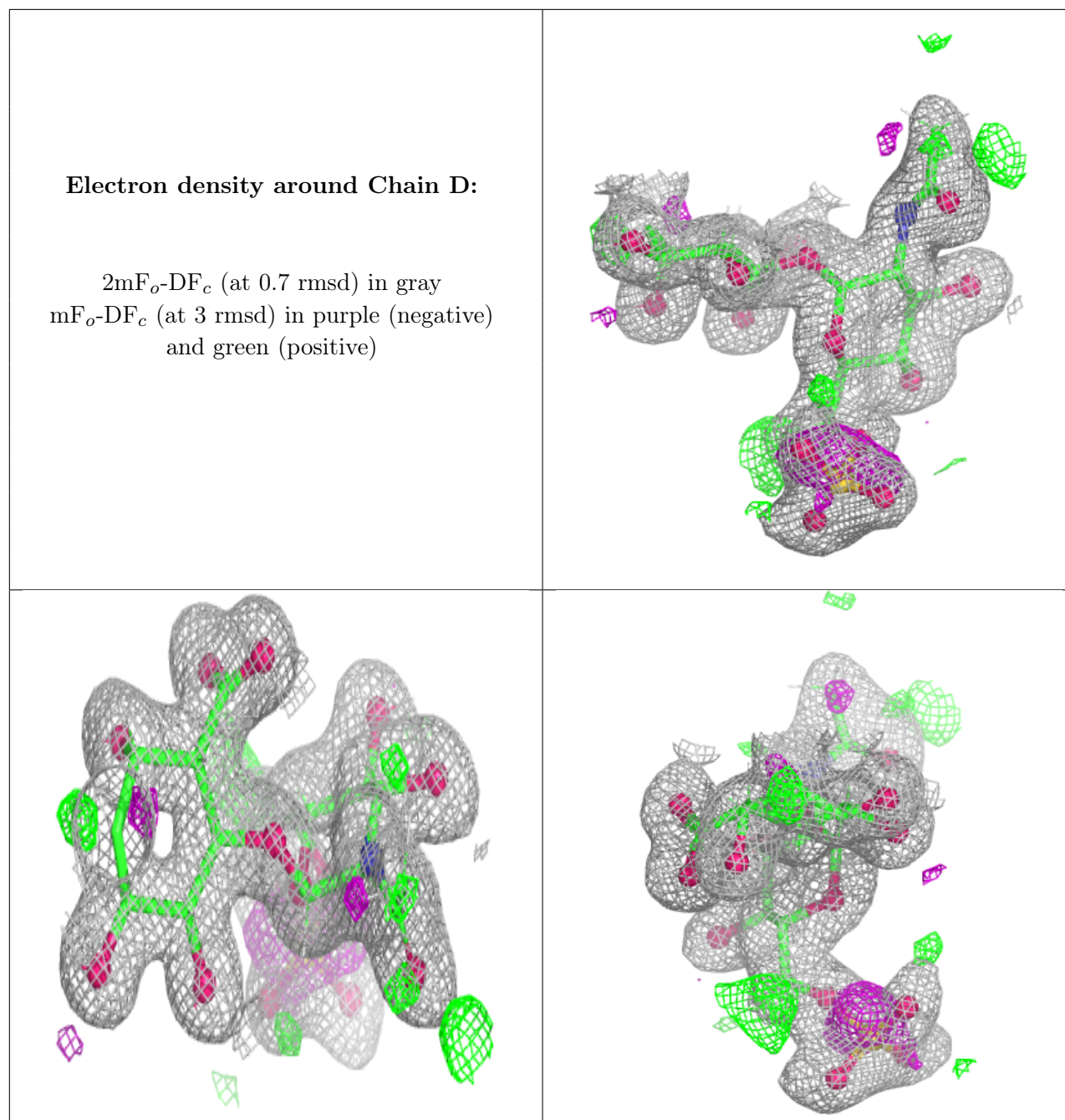
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NGY	D	2	18/19	0.90	0.11	24,28,44,52	2
2	NGY	C	2[B]	18/19	0.94	0.08	15,20,30,32	31
2	NGY	C	2[A]	18/19	0.94	0.08	18,22,32,36	31
2	8I4	D	1	13/14	0.96	0.07	21,22,24,26	3
2	8I4	C	1[A]	13/14	0.98	0.04	15,16,18,19	21
2	8I4	C	1[B]	13/14	0.98	0.04	16,17,17,18	21

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 C:**

$2mF_o-DF_c$  (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(Å <sup>2</sup> )	Q<0.9
3	EDO	A	505	4/4	0.82	0.13	20,32,36,37	1
3	EDO	A	504	4/4	0.83	0.15	20,52,53,53	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	A	502	4/4	0.86	0.13	32,37,38,39	1
3	EDO	B	501	4/4	0.89	0.13	27,34,41,43	1
3	EDO	A	501	4/4	0.93	0.09	30,32,33,33	1
3	EDO	B	502	4/4	0.96	0.07	20,27,31,32	1
3	EDO	A	503	4/4	0.98	0.06	20,21,21,21	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.