



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 04:16 PM BST

PDB ID : 5ERP
Title : Crystal structure of human Desmocollin-2 ectodomain fragment EC2-5
Authors : Harrison, O.J.; Brasch, J.; Shapiro, L.
Deposited on : 2015-11-14
Resolution : 2.70 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

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 : 2.13.1
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) : 2.13.1

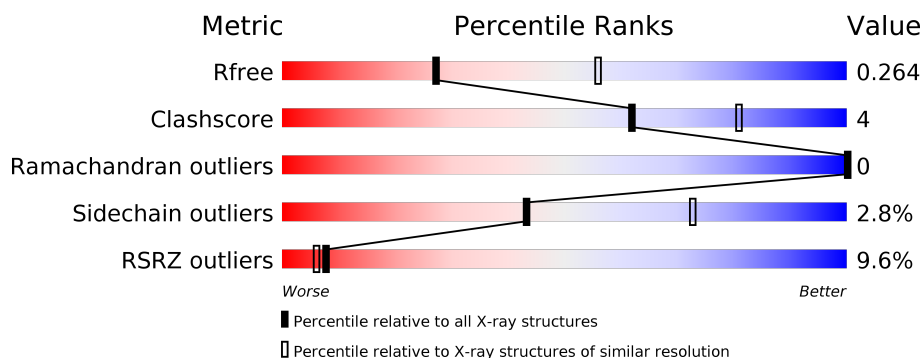
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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 $\leq 5\%$. 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	451	<div> <div>14%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>••</div> </div> </div>
1	B	451	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>•</div> </div> </div>
2	C	4	<div> <div></div> <div> <div>75%</div> <div>25%</div> </div> </div>
2	D	4	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	E	4	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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
5	CA	B	621	-	-	-	X
7	EDO	A	822	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 14287 atoms, of which 6991 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.

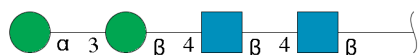
- Molecule 1 is a protein called Desmocollin-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	443	Total	C	H	N	O	S	0	0	0
			6802	2140	3358	575	710	19			
1	B	438	Total	C	H	N	O	S	0	0	0
			6733	2121	3323	569	701	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	546	HIS	-	expression tag	UNP Q02487
A	547	HIS	-	expression tag	UNP Q02487
A	548	HIS	-	expression tag	UNP Q02487
A	549	HIS	-	expression tag	UNP Q02487
A	550	HIS	-	expression tag	UNP Q02487
A	551	HIS	-	expression tag	UNP Q02487
B	546	HIS	-	expression tag	UNP Q02487
B	547	HIS	-	expression tag	UNP Q02487
B	548	HIS	-	expression tag	UNP Q02487
B	549	HIS	-	expression tag	UNP Q02487
B	550	HIS	-	expression tag	UNP Q02487
B	551	HIS	-	expression tag	UNP Q02487

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



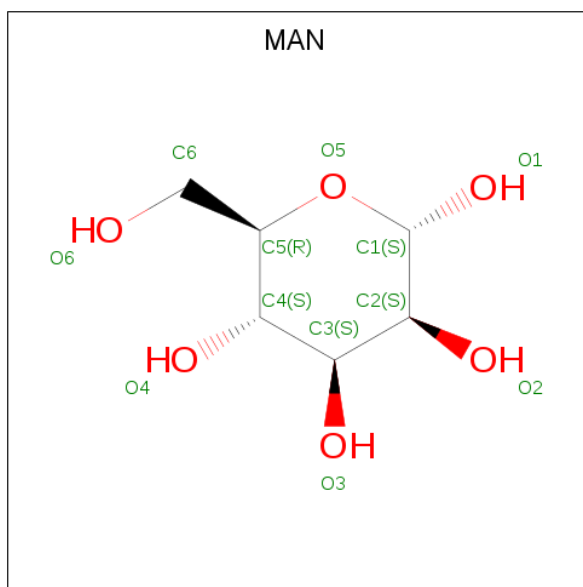
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	4	Total	C	H	N	O	0	0	0
			100	28	50	2	20			

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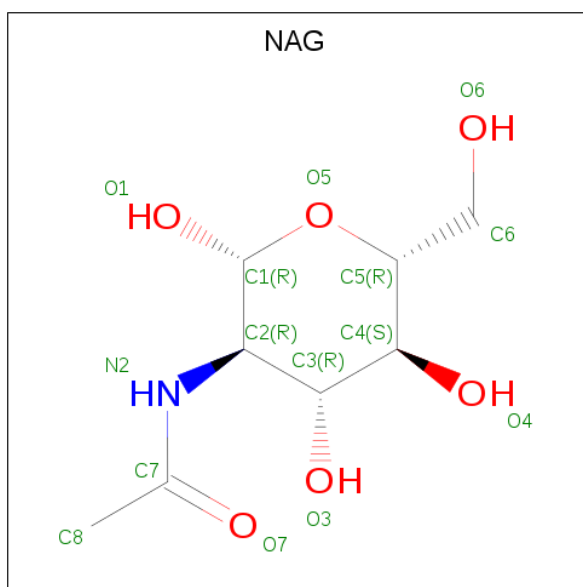
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	4	Total	C	H	N	O	0	0	0
			100	28	50	2	20			
2	E	4	Total	C	H	N	O	0	0	0
			100	28	50	2	20			

- Molecule 3 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			22	6	11	5		
3	A	1	Total	C	H	O	0	0
			22	6	11	5		
3	A	1	Total	C	H	O	0	0
			22	6	11	5		
3	A	1	Total	C	H	O	0	0
			22	6	11	5		
3	B	1	Total	C	H	O	0	0
			22	6	11	5		
3	B	1	Total	C	H	O	0	0
			22	6	11	5		
3	B	1	Total	C	H	O	0	0
			22	6	11	5		
3	B	1	Total	C	H	O	0	0
			22	6	11	5		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

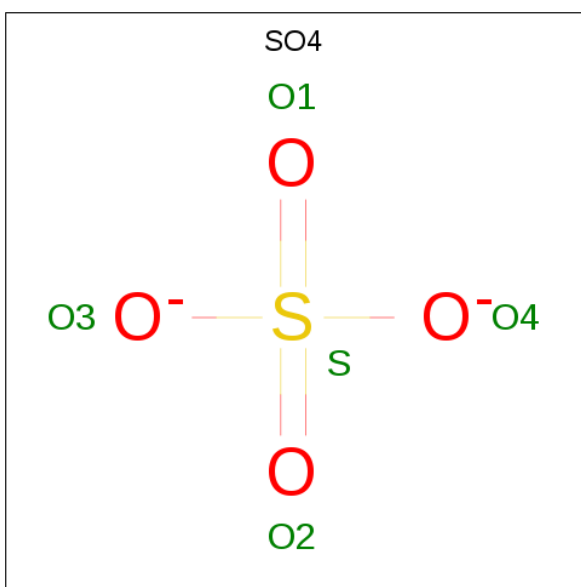


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

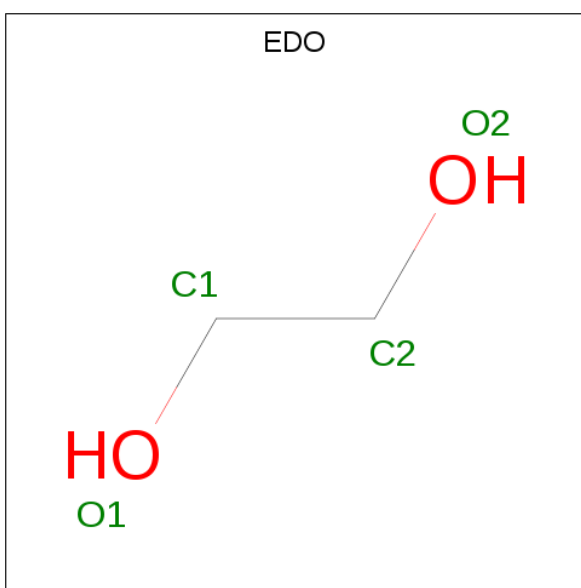
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	11	Total	Ca	0	0
			11	11		
5	A	10	Total	Ca	0	0
			10	10		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

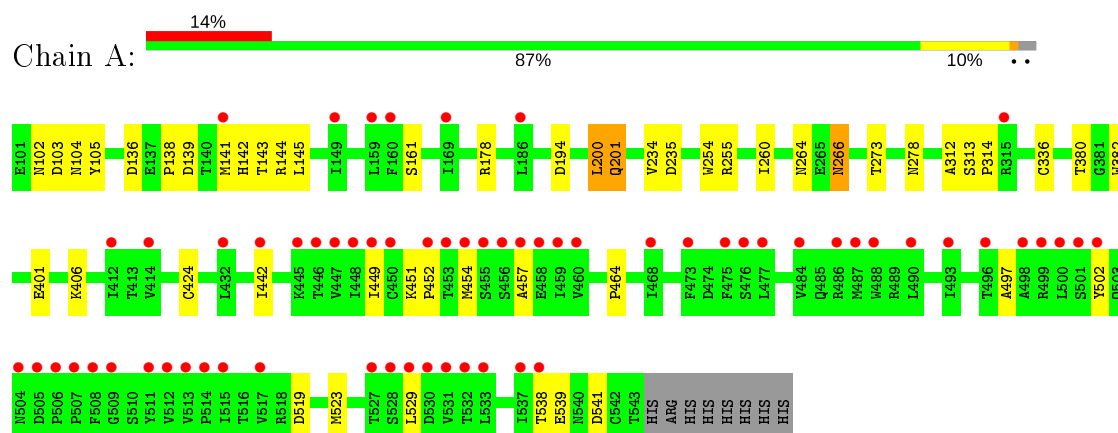
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	59	Total	O	0	0
			59	59		
8	B	52	Total	O	0	0
			52	52		

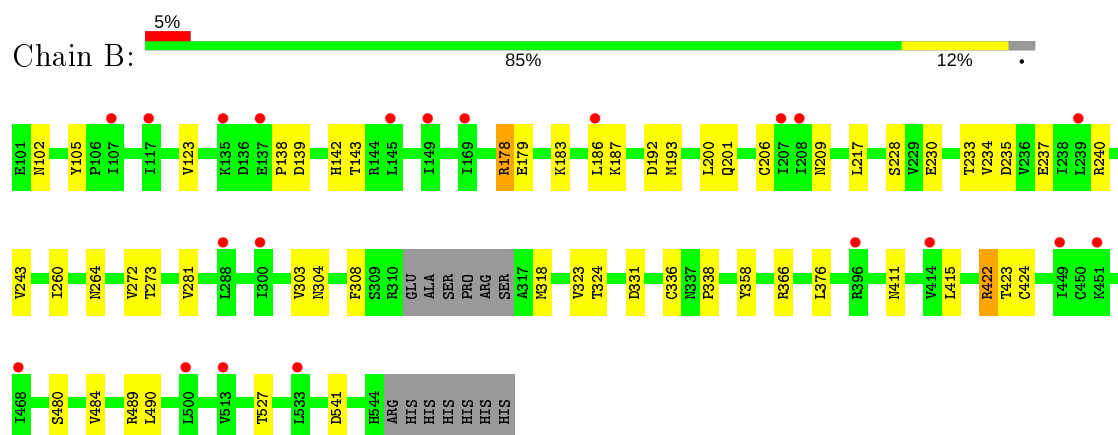
3 Residue-property plots

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.

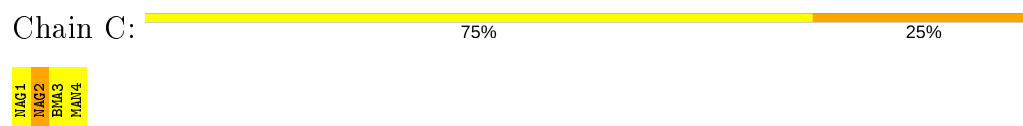
• Molecule 1: Desmocollin-2



• Molecule 1: Desmocollin-2



• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  50% 50%

HA01
HA02
BOA3
MA04

- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 50%

HA01
HA02
BOA3
MA04

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.22Å 94.17Å 126.31Å 90.00° 93.66° 90.00°	Depositor
Resolution (Å)	79.12 – 2.70 79.12 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.4 (79.12-2.70) 86.7 (79.12-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.69Å)	Xtriage
Refinement program	PHENIX dev_1810	Depositor
R, R_{free}	0.224 , 0.262 0.226 , 0.264	Depositor DCC
R_{free} test set	1951 reflections (4.23%)	wwPDB-VP
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14287	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CA, EDO, SO4, MAN

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	0.29	1/3505 (0.0%)	0.52	0/4778
1	B	0.25	0/3470	0.50	0/4729
All	All	0.27	1/6975 (0.0%)	0.51	0/9507

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	497	ALA	CA-CB	5.16	1.63	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3444	3358	3355	28	0
1	B	3410	3323	3321	27	1
2	C	50	50	43	3	0
2	D	50	50	43	0	0
2	E	50	50	43	2	0
3	A	44	44	39	1	0
3	B	44	44	40	2	0
4	A	28	28	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	14	14	13	0	0
5	A	10	0	0	0	0
5	B	11	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	12	18	18	0	0
7	B	8	12	11	1	0
8	A	59	0	0	0	0
8	B	52	0	0	0	0
All	All	7296	6991	6952	62	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 4.

All (62) 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)
3:A:801:MAN:C6	3:A:801:MAN:O6	1.65	1.43
2:E:3:BMA:O2	2:E:4:MAN:O2	2.00	0.76
1:B:336:CYS:N	1:B:424:CYS:SG	2.64	0.71
1:B:192:ASP:OD1	1:B:200:LEU:N	2.29	0.65
1:A:454:MET:O	1:A:502:TYR:OH	2.13	0.63
1:A:336:CYS:N	1:A:424:CYS:SG	2.72	0.62
1:A:141:MET:SD	1:A:144:ARG:NH2	2.72	0.62
1:A:105:TYR:HD1	1:A:200:LEU:HB3	1.65	0.61
2:C:2:NAG:O3	2:C:3:BMA:O5	2.14	0.60
1:A:102:ASN:OD1	1:A:103:ASP:N	2.35	0.59
1:B:183:LYS:HE2	1:B:209:ASN:OD1	2.04	0.58
1:B:138:PRO:HA	1:B:143:THR:HG21	1.88	0.56
1:B:102:ASN:ND2	1:B:193:MET:SD	2.78	0.55
2:C:2:NAG:H83	2:C:2:NAG:H3	1.88	0.55
1:A:449:ILE:HG12	1:A:457:ALA:HB2	1.88	0.55
1:B:331:ASP:O	1:B:422:ARG:NH2	2.40	0.54
1:A:266:ASN:ND2	1:A:266:ASN:O	2.39	0.51
1:A:451:LYS:N	1:A:452:PRO:CD	2.74	0.51
1:B:411:ASN:CG	7:B:627:EDO:H12	2.32	0.50
1:B:178:ARG:NH1	1:B:179:GLU:OE2	2.44	0.50
1:A:519:ASP:OD1	1:A:523:MET:N	2.45	0.50
1:A:538:THR:O	1:A:539:GLU:HB3	2.11	0.49
1:A:141:MET:SD	1:A:194:ASP:HB2	2.53	0.49
1:B:105:TYR:HE1	1:B:200:LEU:HD22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:GLU:O	1:B:233:THR:OG1	2.30	0.48
1:A:102:ASN:HB2	1:A:136:ASP:OD2	2.13	0.48
1:B:187:LYS:HE3	3:B:611:MAN:H2	1.95	0.48
1:A:138:PRO:HA	1:A:143:THR:HG21	1.96	0.48
1:A:102:ASN:HB3	1:A:142:HIS:ND1	2.28	0.47
1:B:338:PRO:O	1:B:358:TYR:OH	2.24	0.47
1:A:380:THR:HG21	1:A:382:TRP:CE2	2.50	0.47
1:B:186:LEU:O	1:B:206:CYS:N	2.47	0.46
1:B:183:LYS:HG3	1:B:209:ASN:OD1	2.16	0.46
1:A:313:SER:N	1:A:314:PRO:HD3	2.31	0.45
1:A:442:ILE:HG21	1:A:529:LEU:HD21	1.99	0.45
1:B:303:VAL:HG12	1:B:304:ASN:N	2.31	0.45
1:A:234:VAL:HG22	1:A:235:ASP:N	2.32	0.45
1:A:260:ILE:HG21	1:A:264:ASN:HB2	1.97	0.45
3:B:610:MAN:HO3	3:B:611:MAN:HO6	1.59	0.44
1:A:105:TYR:CD1	1:A:200:LEU:HB3	2.49	0.44
1:A:312:ALA:C	1:A:314:PRO:HD3	2.38	0.44
1:B:102:ASN:HB3	1:B:142:HIS:HB3	2.00	0.44
1:B:217:LEU:HD13	1:B:308:PHE:CD1	2.53	0.44
1:A:541:ASP:OD2	1:A:541:ASP:N	2.50	0.43
1:B:234:VAL:HG22	1:B:235:ASP:N	2.34	0.43
1:B:240:ARG:HG2	1:B:281:VAL:HG22	2.01	0.43
1:B:541:ASP:N	1:B:541:ASP:OD1	2.52	0.43
1:A:401:GLU:HG2	1:A:464:PRO:HB2	2.00	0.42
1:B:260:ILE:HG21	1:B:264:ASN:HB2	2.01	0.42
1:B:303:VAL:HG23	1:B:318:MET:HE3	2.01	0.42
2:E:3:BMA:O2	2:E:4:MAN:C2	2.67	0.42
1:B:237:GLU:HB2	1:B:281:VAL:CG1	2.50	0.42
1:A:201:GLN:NE2	1:A:201:GLN:O	2.53	0.42
1:B:415:LEU:HD11	1:B:423:THR:HB	2.02	0.42
1:A:406:LYS:H	2:C:1:NAG:H83	1.84	0.42
1:B:480:SER:HB2	1:B:484:VAL:CG2	2.51	0.41
1:A:104:ASN:HB2	1:A:136:ASP:OD2	2.20	0.41
4:A:810:NAG:H3	4:A:810:NAG:H83	2.03	0.41
1:B:105:TYR:CE1	1:B:200:LEU:HD22	2.55	0.41
1:B:490:LEU:O	1:B:490:LEU:HD12	2.20	0.41
1:A:254:TRP:CH2	1:A:278:ASN:HB2	2.55	0.41
1:A:312:ALA:HB1	1:A:314:PRO:HD3	2.02	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)
1:B:228:SER:O	1:B:489:ARG:NH2[3_555]	2.18	0.02

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	441/451 (98%)	416 (94%)	25 (6%)	0	100	100
1	B	434/451 (96%)	410 (94%)	24 (6%)	0	100	100
All	All	875/902 (97%)	826 (94%)	49 (6%)	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	402/410 (98%)	393 (98%)	9 (2%)	52	79
1	B	398/410 (97%)	385 (97%)	13 (3%)	38	67
All	All	800/820 (98%)	778 (97%)	22 (3%)	43	73

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	ASP
1	A	145	LEU
1	A	161	SER

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Mol	Chain	Res	Type
1	A	178	ARG
1	A	200	LEU
1	A	201	GLN
1	A	255	ARG
1	A	266	ASN
1	A	273	THR
1	B	123	VAL
1	B	139	ASP
1	B	178	ARG
1	B	201	GLN
1	B	243	VAL
1	B	272	VAL
1	B	273	THR
1	B	323	VAL
1	B	324	THR
1	B	366	ARG
1	B	376	LEU
1	B	422	ARG
1	B	527	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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	NAG	C	1	1,2	14,14,15	0.19	0	17,19,21	0.59	0
2	NAG	C	2	2	14,14,15	0.30	0	17,19,21	1.07	2 (11%)
2	BMA	C	3	2	11,11,12	0.69	0	15,15,17	0.76	0
2	MAN	C	4	2	11,11,12	0.66	0	15,15,17	0.94	1 (6%)
2	NAG	D	1	1,2	14,14,15	1.89	3 (21%)	17,19,21	1.11	2 (11%)
2	NAG	D	2	2	14,14,15	0.41	0	17,19,21	0.60	0
2	BMA	D	3	2	11,11,12	0.81	0	15,15,17	0.85	0
2	MAN	D	4	2	11,11,12	0.78	0	15,15,17	1.00	2 (13%)
2	NAG	E	1	1,2	14,14,15	0.30	0	17,19,21	0.61	0
2	NAG	E	2	2	14,14,15	0.25	0	17,19,21	0.54	0
2	BMA	E	3	2	11,11,12	1.53	3 (27%)	15,15,17	1.50	4 (26%)
2	MAN	E	4	2	11,11,12	1.03	1 (9%)	15,15,17	2.25	4 (26%)

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	NAG	C	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	C	2	2	-	6/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	1/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	MAN	D	4	2	-	1/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	O5-C1	5.89	1.53	1.43
2	E	3	BMA	O3-C3	3.16	1.50	1.43
2	E	4	MAN	C1-C2	2.67	1.58	1.52
2	D	1	NAG	C1-C2	2.59	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	BMA	C1-C2	-2.15	1.47	1.52
2	E	3	BMA	O5-C5	2.05	1.47	1.43
2	D	1	NAG	C8-C7	2.03	1.54	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4	MAN	C1-C2-C3	5.43	116.34	109.67
2	E	3	BMA	C1-O5-C5	3.99	117.59	112.19
2	E	4	MAN	C1-O5-C5	3.94	117.54	112.19
2	E	4	MAN	O2-C2-C3	-3.94	102.24	110.14
2	C	2	NAG	C2-N2-C7	3.39	127.73	122.90
2	E	4	MAN	O5-C1-C2	2.59	114.76	110.77
2	E	3	BMA	O3-C3-C2	2.48	114.74	109.99
2	D	1	NAG	C1-O5-C5	-2.29	109.10	112.19
2	D	4	MAN	O2-C2-C3	-2.26	105.62	110.14
2	D	4	MAN	C1-O5-C5	2.20	115.18	112.19
2	E	3	BMA	O2-C2-C1	-2.19	104.68	109.15
2	C	4	MAN	O2-C2-C3	-2.17	105.79	110.14
2	D	1	NAG	O5-C5-C6	2.10	110.50	107.20
2	C	2	NAG	C1-C2-N2	2.05	113.99	110.49
2	E	3	BMA	O3-C3-C4	2.04	115.07	110.35

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	4	MAN	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	E	3	BMA	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	D	4	MAN	O5-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6

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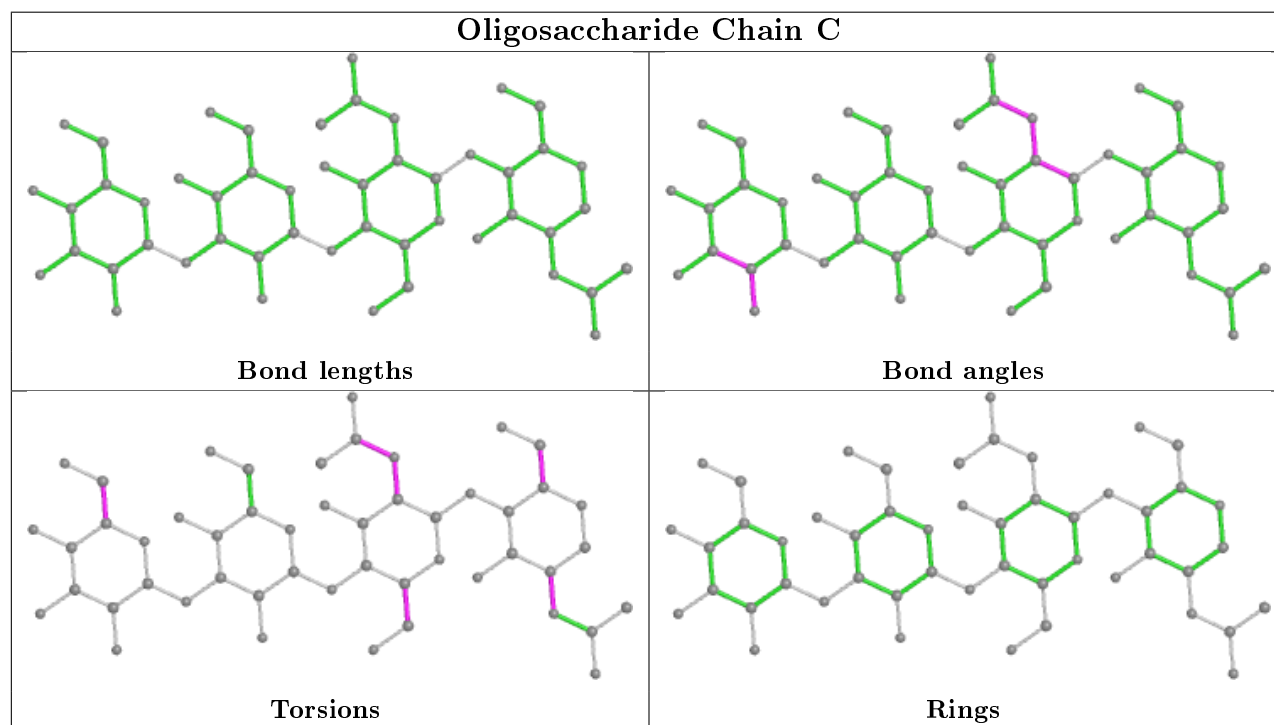
Mol	Chain	Res	Type	Atoms
2	E	3	BMA	C4-C5-C6-O6
2	C	1	NAG	C1-C2-N2-C7
2	C	2	NAG	C3-C2-N2-C7
2	C	2	NAG	C1-C2-N2-C7

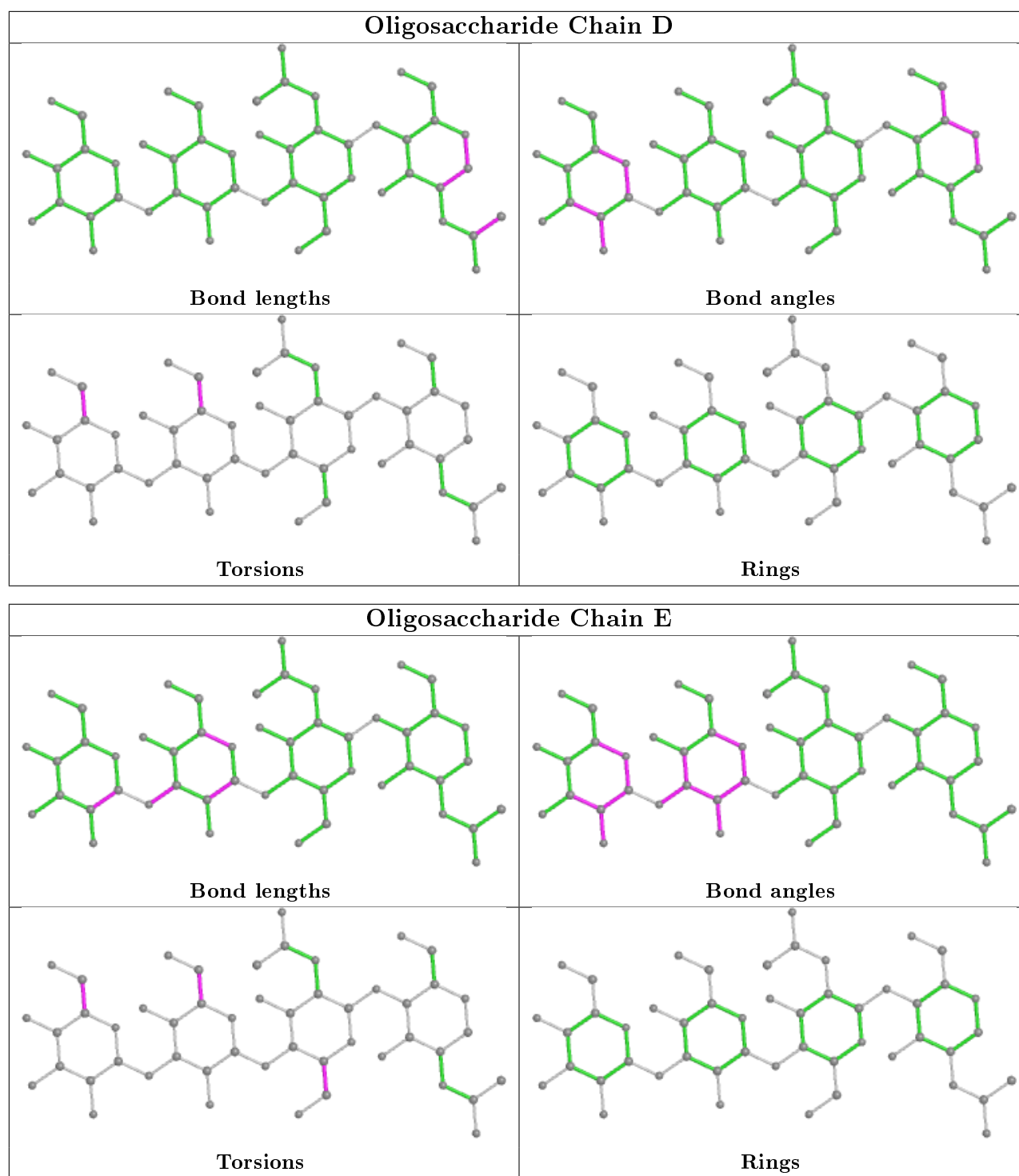
There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	4	MAN	2	0
2	C	3	BMA	1	0
2	E	3	BMA	2	0
2	C	2	NAG	2	0
2	C	1	NAG	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](#)

Of 39 ligands modelled in this entry, 21 are monoatomic - leaving 18 for Mogul analysis.

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
4	NAG	B	601	1	14,14,15	0.50	0	17,19,21	0.66	1 (5%)
3	MAN	A	801	1	11,11,12	2.08	3 (27%)	15,15,17	2.82	4 (26%)
3	MAN	B	612	1	11,11,12	0.92	1 (9%)	15,15,17	1.28	2 (13%)
4	NAG	A	805	1	14,14,15	1.08	2 (14%)	17,19,21	1.00	1 (5%)
7	EDO	B	627	-	3,3,3	0.69	0	2,2,2	2.10	1 (50%)
3	MAN	B	613	1	11,11,12	0.72	0	15,15,17	1.99	4 (26%)
7	EDO	A	824	-	3,3,3	0.45	0	2,2,2	0.31	0
7	EDO	B	626	-	3,3,3	0.44	0	2,2,2	0.29	0
3	MAN	A	802	1	11,11,12	0.88	1 (9%)	15,15,17	1.56	3 (20%)
4	NAG	A	810	1	14,14,15	1.70	1 (7%)	17,19,21	1.56	4 (23%)
3	MAN	A	803	1	11,11,12	0.94	1 (9%)	15,15,17	1.09	1 (6%)
3	MAN	B	610	1	11,11,12	0.68	0	15,15,17	1.28	2 (13%)
3	MAN	A	804	1	11,11,12	0.93	1 (9%)	15,15,17	1.01	1 (6%)
7	EDO	A	822	-	3,3,3	0.44	0	2,2,2	0.44	0
6	SO4	A	821	-	4,4,4	0.14	0	6,6,6	0.05	0
3	MAN	B	611	1	11,11,12	0.69	0	15,15,17	1.33	3 (20%)
7	EDO	A	823	-	3,3,3	0.44	0	2,2,2	0.33	0
6	SO4	B	625	-	4,4,4	0.14	0	6,6,6	0.06	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
4	NAG	B	601	1	-	2/6/23/26	0/1/1/1
3	MAN	A	801	1	-	0/2/19/22	0/1/1/1
3	MAN	B	612	1	-	1/2/19/22	0/1/1/1
4	NAG	A	805	1	-	1/6/23/26	0/1/1/1
7	EDO	B	627	-	-	0/1/1/1	-
3	MAN	B	613	1	-	0/2/19/22	0/1/1/1
7	EDO	A	824	-	-	0/1/1/1	-
7	EDO	B	626	-	-	1/1/1/1	-
3	MAN	A	802	1	-	0/2/19/22	1/1/1/1
4	NAG	A	810	1	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	A	803	1	-	0/2/19/22	0/1/1/1
3	MAN	B	610	1	-	0/2/19/22	0/1/1/1
3	MAN	A	804	1	-	1/2/19/22	0/1/1/1
7	EDO	A	822	-	-	1/1/1/1	-
3	MAN	B	611	1	-	0/2/19/22	1/1/1/1
7	EDO	A	823	-	-	0/1/1/1	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	810	NAG	O5-C1	6.13	1.53	1.43
3	A	801	MAN	O6-C6	5.57	1.65	1.42
4	A	805	NAG	O5-C1	3.29	1.49	1.43
3	A	801	MAN	O5-C1	-2.48	1.39	1.43
3	B	612	MAN	O5-C5	2.43	1.48	1.43
4	A	805	NAG	C1-C2	2.27	1.55	1.52
3	A	804	MAN	O5-C1	-2.12	1.40	1.43
3	A	801	MAN	O5-C5	2.05	1.47	1.43
3	A	802	MAN	O5-C1	-2.03	1.40	1.43
3	A	803	MAN	O5-C1	-2.01	1.40	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	MAN	C1-O5-C5	9.37	124.89	112.19
3	B	613	MAN	C1-O5-C5	4.64	118.48	112.19
3	A	802	MAN	C1-O5-C5	4.53	118.33	112.19
3	B	613	MAN	O5-C1-C2	4.37	117.52	110.77
3	A	801	MAN	O5-C1-C2	3.75	116.56	110.77
3	B	612	MAN	C1-O5-C5	3.64	117.12	112.19
4	A	810	NAG	C2-N2-C7	3.62	128.06	122.90
3	B	611	MAN	C1-O5-C5	3.45	116.87	112.19
4	A	810	NAG	C1-O5-C5	3.44	116.85	112.19
4	A	805	NAG	C1-O5-C5	3.31	116.68	112.19
3	B	610	MAN	C1-O5-C5	3.31	116.67	112.19
3	B	613	MAN	C1-C2-C3	2.79	113.10	109.67
3	A	803	MAN	C1-O5-C5	2.49	115.57	112.19
4	A	810	NAG	C1-C2-N2	2.49	114.75	110.49
3	B	611	MAN	O2-C2-C1	2.44	114.14	109.15
3	A	802	MAN	O2-C2-C3	-2.43	105.28	110.14
4	B	601	NAG	C1-O5-C5	2.38	115.42	112.19
3	A	802	MAN	O5-C1-C2	2.36	114.42	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	627	EDO	O2-C2-C1	-2.31	95.32	111.91
3	B	610	MAN	O2-C2-C3	-2.29	105.55	110.14
3	B	613	MAN	O2-C2-C3	-2.23	105.67	110.14
4	A	810	NAG	C4-C3-C2	-2.20	107.79	111.02
3	B	611	MAN	O2-C2-C3	-2.20	105.73	110.14
3	A	804	MAN	O2-C2-C3	-2.13	105.88	110.14
3	A	801	MAN	O2-C2-C3	-2.09	105.96	110.14
3	A	801	MAN	C6-C5-C4	-2.07	108.17	113.00
3	B	612	MAN	O2-C2-C3	-2.01	106.11	110.14

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	NAG	O5-C5-C6-O6
4	A	810	NAG	C8-C7-N2-C2
4	A	810	NAG	O7-C7-N2-C2
4	B	601	NAG	C4-C5-C6-O6
4	A	810	NAG	O5-C5-C6-O6
7	B	626	EDO	O1-C1-C2-O2
4	A	805	NAG	C3-C2-N2-C7
7	A	822	EDO	O1-C1-C2-O2
4	A	810	NAG	C1-C2-N2-C7
3	A	804	MAN	C4-C5-C6-O6
4	A	810	NAG	C3-C2-N2-C7
3	B	612	MAN	C4-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	MAN	C1-C2-C3-C4-C5-O5
3	B	611	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	MAN	1	0
7	B	627	EDO	1	0
4	A	810	NAG	1	0
3	B	610	MAN	1	0
3	B	611	MAN	2	0

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 ⓘ

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	443/451 (98%)	0.90	64 (14%) 2 1	63, 89, 199, 224	0
1	B	438/451 (97%)	0.54	21 (4%) 30 28	61, 84, 124, 165	0
All	All	881/902 (97%)	0.72	85 (9%) 8 6	61, 86, 187, 224	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	511	TYR	12.6
1	A	531	VAL	9.7
1	A	529	LEU	9.6
1	A	513	VAL	9.1
1	A	533	LEU	8.8
1	A	528	SER	8.3
1	A	487	MET	7.7
1	A	500	LEU	7.4
1	A	515	ILE	6.9
1	A	477	LEU	6.8
1	A	459	ILE	6.5
1	A	505	ASP	6.4
1	A	512	VAL	6.3
1	A	449	ILE	6.2
1	A	454	MET	6.0
1	A	488	TRP	5.8
1	A	456	SER	5.5
1	A	457	ALA	5.5
1	A	530	ASP	5.2
1	A	455	SER	5.1
1	A	499	ARG	5.0
1	A	448	ILE	4.9
1	A	504	ASN	4.9
1	A	506	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	453	THR	4.7
1	A	447	VAL	4.5
1	A	538	THR	4.4
1	A	532	THR	3.7
1	A	412	ILE	3.7
1	A	460	VAL	3.6
1	A	493	ILE	3.5
1	B	396	ARG	3.5
1	A	446	THR	3.4
1	A	527	THR	3.3
1	B	186	LEU	3.3
1	A	502	TYR	3.3
1	B	207	ILE	3.2
1	A	517	VAL	3.2
1	A	501	SER	3.2
1	A	507	PRO	3.2
1	A	508	PHE	3.2
1	A	496	THR	3.1
1	A	514	PRO	3.1
1	A	486	ARG	3.1
1	A	445	LYS	3.0
1	B	533	LEU	3.0
1	A	498	ALA	3.0
1	A	169	ILE	2.9
1	A	473	PHE	2.8
1	A	186	LEU	2.7
1	B	468	ILE	2.7
1	A	484	VAL	2.7
1	B	451	LYS	2.7
1	A	432	LEU	2.7
1	A	458	GLU	2.6
1	A	476	SER	2.6
1	A	537	ILE	2.6
1	B	449	ILE	2.6
1	A	450	CYS	2.6
1	A	475	PHE	2.5
1	B	107	ILE	2.5
1	A	442	ILE	2.5
1	A	509	GLY	2.4
1	B	117	ILE	2.4
1	B	169	ILE	2.4
1	A	160	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	141	MET	2.3
1	B	300	ILE	2.3
1	B	288	LEU	2.2
1	A	468	ILE	2.1
1	B	414	VAL	2.1
1	B	239	LEU	2.1
1	A	315	ARG	2.1
1	B	149	ILE	2.1
1	A	452	PRO	2.1
1	B	137	GLU	2.1
1	A	149	ILE	2.1
1	B	145	LEU	2.1
1	B	500	LEU	2.1
1	A	159	LEU	2.1
1	A	414	VAL	2.1
1	B	135	LYS	2.1
1	A	490	LEU	2.0
1	B	513	VAL	2.0
1	B	208	ILE	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, 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.

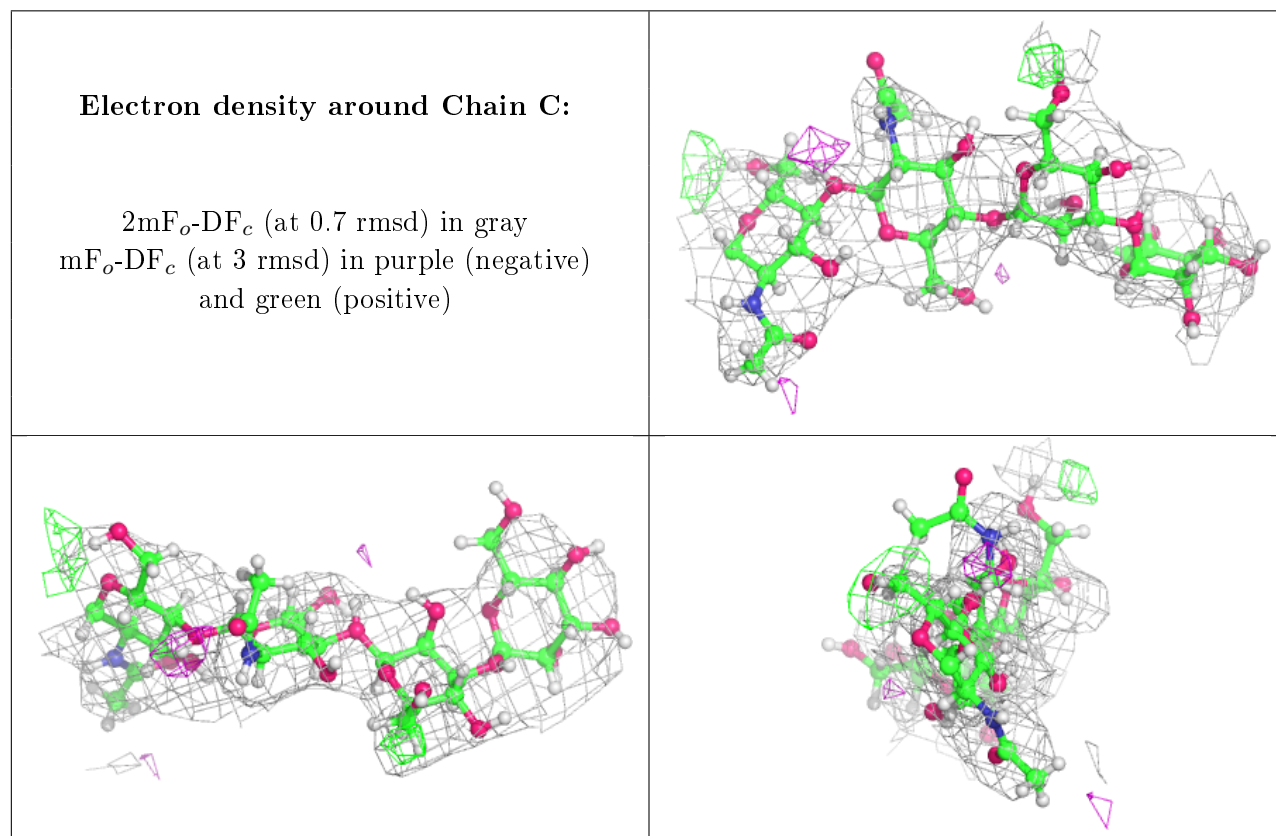
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	C	3	11/12	0.73	0.17	177,195,231,234	0
2	MAN	E	4	11/12	0.79	0.15	164,186,218,222	0
2	MAN	D	4	11/12	0.81	0.14	150,172,202,207	0
2	MAN	C	4	11/12	0.82	0.17	181,206,242,247	0
2	BMA	E	3	11/12	0.84	0.12	158,185,213,222	0
2	BMA	D	3	11/12	0.87	0.10	145,170,196,200	0
2	NAG	C	2	14/15	0.88	0.25	138,166,193,202	0
2	NAG	D	2	14/15	0.89	0.15	96,124,161,193	0
2	NAG	D	1	14/15	0.89	0.15	82,117,141,157	0

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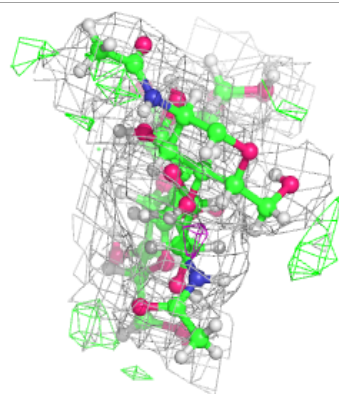
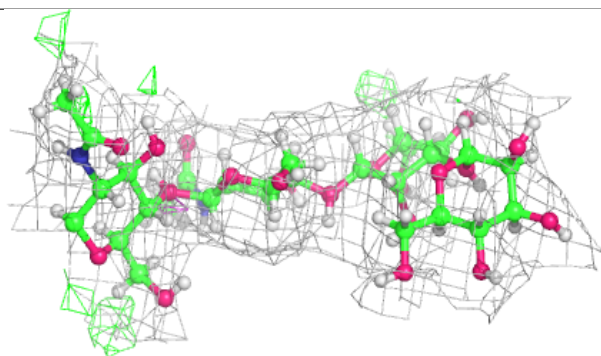
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	C	1	14/15	0.91	0.19	94,124,152,159	0
2	NAG	E	2	14/15	0.92	0.15	93,130,163,184	0
2	NAG	E	1	14/15	0.93	0.18	72,100,134,151	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

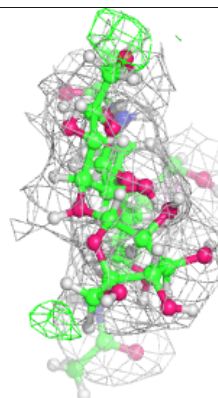
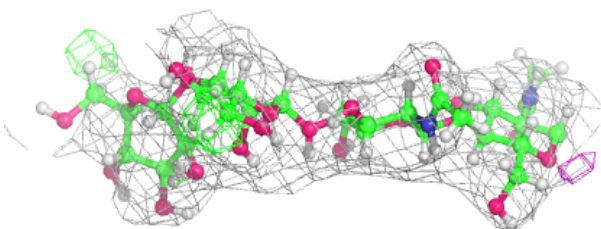
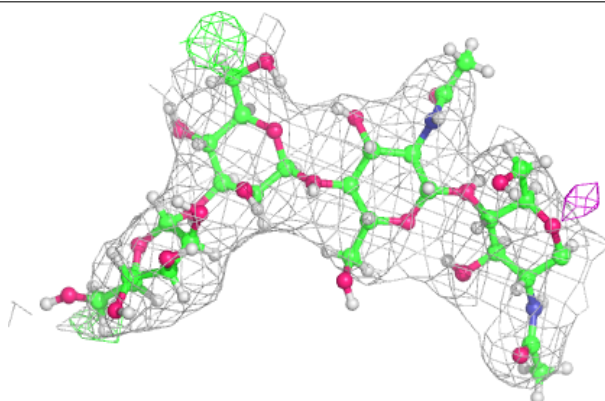


Electron density around Chain D:

$2mF_o-DF_c$ (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 ⓘ

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
5	CA	B	621	1/1	0.49	0.49	217,217,217,217	0
7	EDO	A	824	4/4	0.51	0.34	98,118,122,133	0
7	EDO	A	823	4/4	0.62	0.21	135,162,168,168	0
7	EDO	A	822	4/4	0.73	0.72	106,128,132,132	0
7	EDO	B	626	4/4	0.80	0.23	92,110,126,126	0
4	NAG	A	805	14/15	0.81	0.16	121,149,181,193	0
5	CA	A	817	1/1	0.81	0.31	119,119,119,119	0
3	MAN	A	801	11/12	0.83	0.22	114,136,159,176	0
4	NAG	A	810	14/15	0.83	0.10	164,197,226,234	0
6	SO4	B	625	5/5	0.84	0.24	139,141,148,165	0
3	MAN	B	611	11/12	0.85	0.19	124,149,179,185	0
5	CA	B	614	1/1	0.86	0.21	103,103,103,103	0
3	MAN	A	804	11/12	0.88	0.25	113,147,171,194	0
4	NAG	B	601	14/15	0.88	0.14	99,123,145,155	0
7	EDO	B	627	4/4	0.89	0.33	97,132,142,158	0
3	MAN	B	613	11/12	0.89	0.27	124,149,178,179	0
3	MAN	B	612	11/12	0.89	0.33	116,143,183,187	0
3	MAN	A	802	11/12	0.90	0.21	108,133,157,166	0
5	CA	B	624	1/1	0.91	0.11	119,119,119,119	0
6	SO4	A	821	5/5	0.91	0.08	150,154,165,171	0
5	CA	A	820	1/1	0.91	0.24	123,123,123,123	0
5	CA	B	623	1/1	0.92	0.36	102,102,102,102	0
3	MAN	A	803	11/12	0.92	0.20	94,119,141,144	0
3	MAN	B	610	11/12	0.94	0.17	117,146,169,179	0
5	CA	A	813	1/1	0.95	0.28	76,76,76,76	0
5	CA	B	620	1/1	0.95	0.25	92,92,92,92	0
5	CA	B	616	1/1	0.95	0.22	91,91,91,91	0
5	CA	A	814	1/1	0.95	0.29	83,83,83,83	0
5	CA	B	615	1/1	0.95	0.27	81,81,81,81	0
5	CA	B	619	1/1	0.95	0.29	77,77,77,77	0
5	CA	A	811	1/1	0.95	0.30	116,116,116,116	0
5	CA	A	818	1/1	0.96	0.26	110,110,110,110	0
5	CA	B	622	1/1	0.96	0.30	76,76,76,76	0
5	CA	A	819	1/1	0.96	0.25	86,86,86,86	0
5	CA	A	816	1/1	0.98	0.25	74,74,74,74	0
5	CA	A	815	1/1	0.99	0.27	72,72,72,72	0
5	CA	B	617	1/1	0.99	0.23	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CA	B	618	1/1	0.99	0.27	72,72,72,72	0
5	CA	A	812	1/1	0.99	0.28	81,81,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.