



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:09 PM EDT

PDB ID : 5ERP / pdb_00005erp
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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)
Xtriage (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

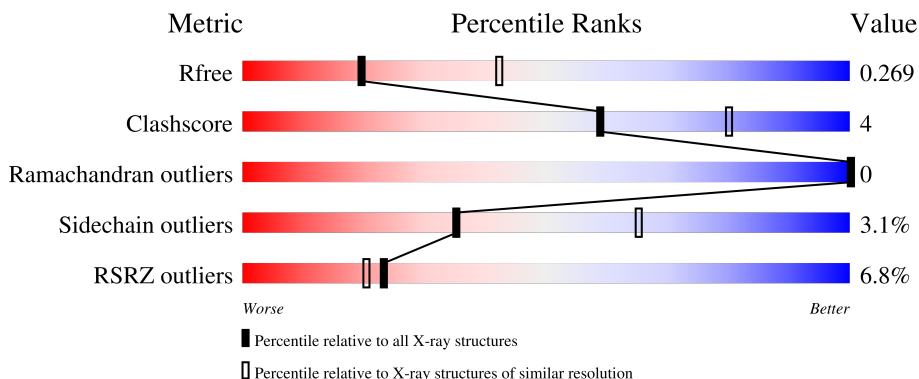
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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 $\leq 5\%$. 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	11% 86% 11% ..
1	B	451	3% 85% 12% ..
2	C	4	75% 25%
2	D	4	50% 50%
2	E	4	50% 50%

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.



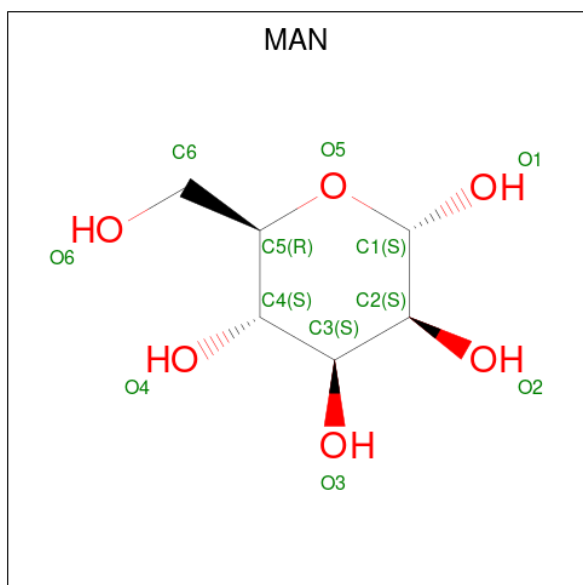
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	4	Total	C	H	N	O	0	0	0
			100	28	50	2	20			

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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 (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



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		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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 (CCD ID: CA) (formula: Ca).

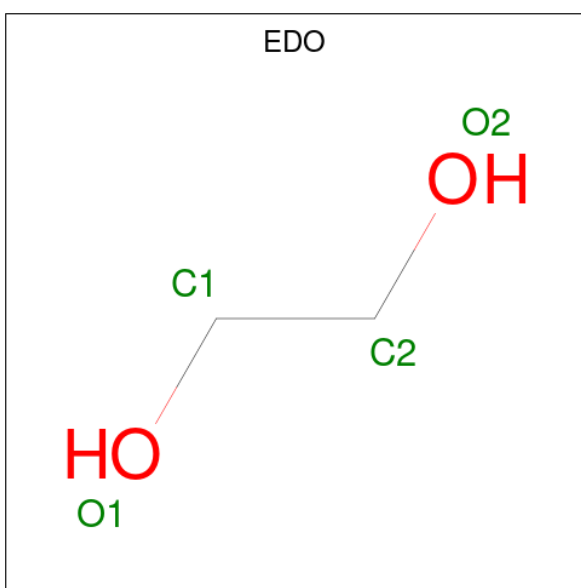
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	Ca	0	0
			10	10		
5	B	11	Total	Ca	0	0
			11	11		

- Molecule 6 is SULFATE ION (CCD ID: 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 (CCD ID: 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		

- Molecule 1: Desmocollin-2



Chain D:  50% 50%



- 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%



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 0.233 , 0.269	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)	0.35 , 52.8	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: CA, NAG, MAN, SO4, BMA, 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	0.35	1/3505 (0.0%)	0.70	3/4778 (0.1%)
1	B	0.34	0/3470	0.68	0/4729
All	All	0.35	1/6975 (0.0%)	0.69	3/9507 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	497	ALA	CA-CB	6.50	1.63	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	ARG	N-CA-C	5.35	117.53	111.11
1	A	411	ASN	N-CA-C	5.19	117.70	109.24
1	A	497	ALA	N-CA-C	-5.18	102.02	110.20

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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:O6	3:A:801:MAN:C6	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:A:454:MET:O	1:A:502:TYR:OH	2.13	0.67
1:B:192:ASP:OD1	1:B:200:LEU:N	2.29	0.65
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:H3	2:C:2:NAG:H83	1.88	0.55
1:B:411:ASN:CG	7:B:619:EDO:H12	2.32	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:O	1:A:266:ASN:ND2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:LYS:N	1:A:452:PRO:CD	2.74	0.51
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:A:312:ALA:C	1:A:314:PRO:HD3	2.38	0.49
1:B:105:TYR:HE1	1:B:200:LEU:HD22	1.77	0.49
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:603: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
1:B:104:ASN:HB2	1:B:136:ASP:CG	2.41	0.45
1:A:105:TYR:CD1	1:A:200:LEU:HB3	2.49	0.44
3:B:602:MAN:HO3	3:B:603:MAN:HO6	1.62	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
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:O	1:A:201:GLN:NE2	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:806:NAG:H83	4:A:806:NAG:H3	2.03	0.41
1:B:105:TYR:CE1	1:B:200:LEU:HD22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:LEU:HD12	1:B:490:LEU:O	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%)	391 (97%)	11 (3%)	39	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	398/410 (97%)	384 (96%)	14 (4%)	32	61
All	All	800/820 (98%)	775 (97%)	25 (3%)	35	65

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	VAL
1	A	139	ASP
1	A	145	LEU
1	A	200	LEU
1	A	201	GLN
1	A	255	ARG
1	A	266	ASN
1	A	273	THR
1	A	318	MET
1	A	374	LYS
1	A	431	ILE
1	B	123	VAL
1	B	193	MET
1	B	201	GLN
1	B	217	LEU
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	380	THR
1	B	422	ARG
1	B	527	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	GLN
1	A	407	ASN
1	A	438	ASN
1	A	503	GLN
1	A	504	ASN
1	B	196	GLN

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Mol	Chain	Res	Type
1	B	299	GLN
1	B	407	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 ⓘ

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	0.61	0
2	NAG	C	2	2	14,14,15	0.31	0	17,19,21	1.14	2 (11%)
2	BMA	C	3	2	11,11,12	0.67	0	15,15,17	0.70	0
2	MAN	C	4	2	11,11,12	0.64	0	15,15,17	0.91	1 (6%)
2	NAG	D	1	1,2	14,14,15	1.86	3 (21%)	17,19,21	1.05	1 (5%)
2	NAG	D	2	2	14,14,15	0.41	0	17,19,21	0.61	0
2	BMA	D	3	2	11,11,12	0.78	0	15,15,17	0.83	0
2	MAN	D	4	2	11,11,12	0.75	0	15,15,17	0.97	2 (13%)
2	NAG	E	1	1,2	14,14,15	0.31	0	17,19,21	0.62	0
2	NAG	E	2	2	14,14,15	0.24	0	17,19,21	0.56	0
2	BMA	E	3	2	11,11,12	1.49	3 (27%)	15,15,17	1.45	2 (13%)
2	MAN	E	4	2	11,11,12	1.00	1 (9%)	15,15,17	2.03	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	2/6/23/26	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	5.61	1.53	1.43
2	E	3	BMA	O3-C3	3.02	1.50	1.43
2	D	1	NAG	C1-C2	2.83	1.56	1.52
2	E	4	MAN	C1-C2	2.55	1.58	1.52
2	E	3	BMA	O5-C5	2.14	1.47	1.43
2	E	3	BMA	C1-C2	-2.05	1.47	1.52
2	D	1	NAG	C8-C7	2.03	1.54	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4	MAN	C1-C2-C3	4.60	116.34	109.64
2	E	3	BMA	C1-O5-C5	4.04	117.59	112.19
2	E	4	MAN	C1-O5-C5	3.99	117.54	112.19
2	E	4	MAN	O2-C2-C3	-3.82	102.24	110.15
2	C	2	NAG	C2-N2-C7	3.60	127.73	122.90
2	D	1	NAG	C1-O5-C5	-2.31	109.10	112.19
2	E	3	BMA	O3-C3-C2	2.30	114.74	110.05
2	C	2	NAG	C1-C2-N2	2.26	113.99	110.43
2	D	4	MAN	C1-O5-C5	2.23	115.18	112.19
2	D	4	MAN	O2-C2-C3	-2.19	105.62	110.15
2	C	4	MAN	O2-C2-C3	-2.11	105.79	110.15

There are no chirality outliers.

All (18) torsion outliers are listed below:

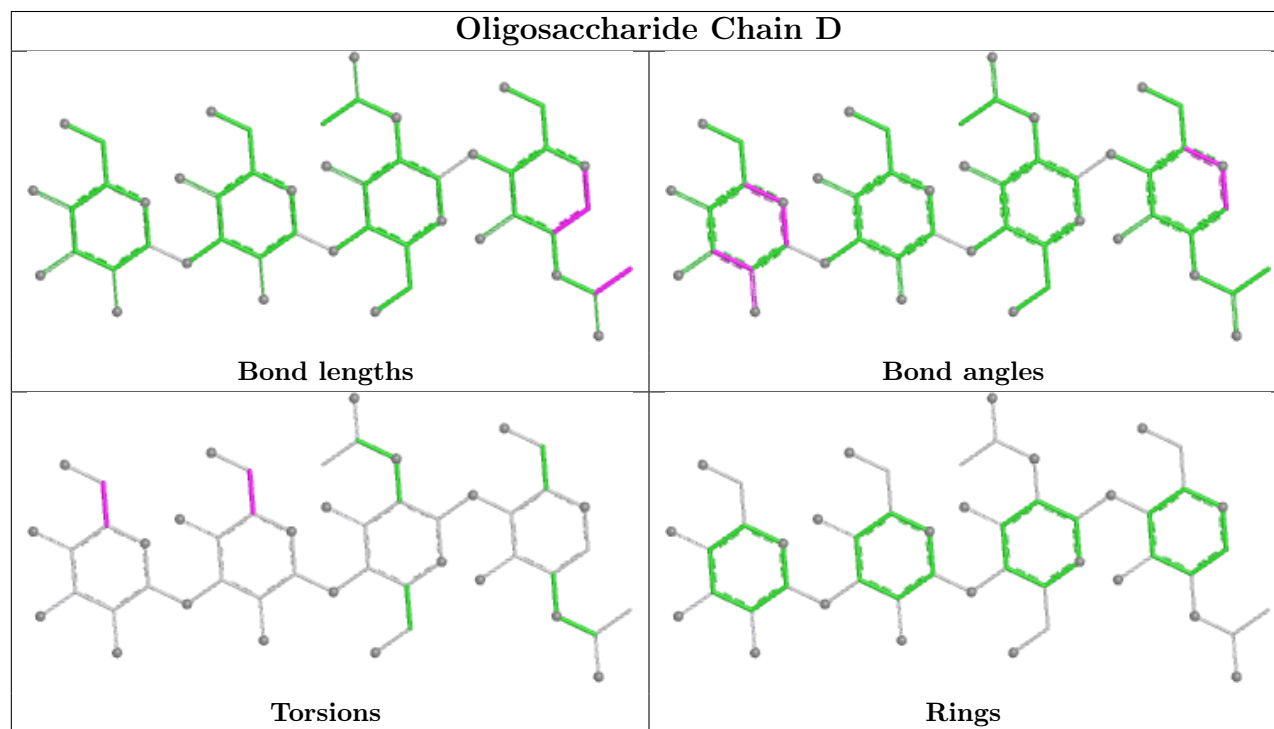
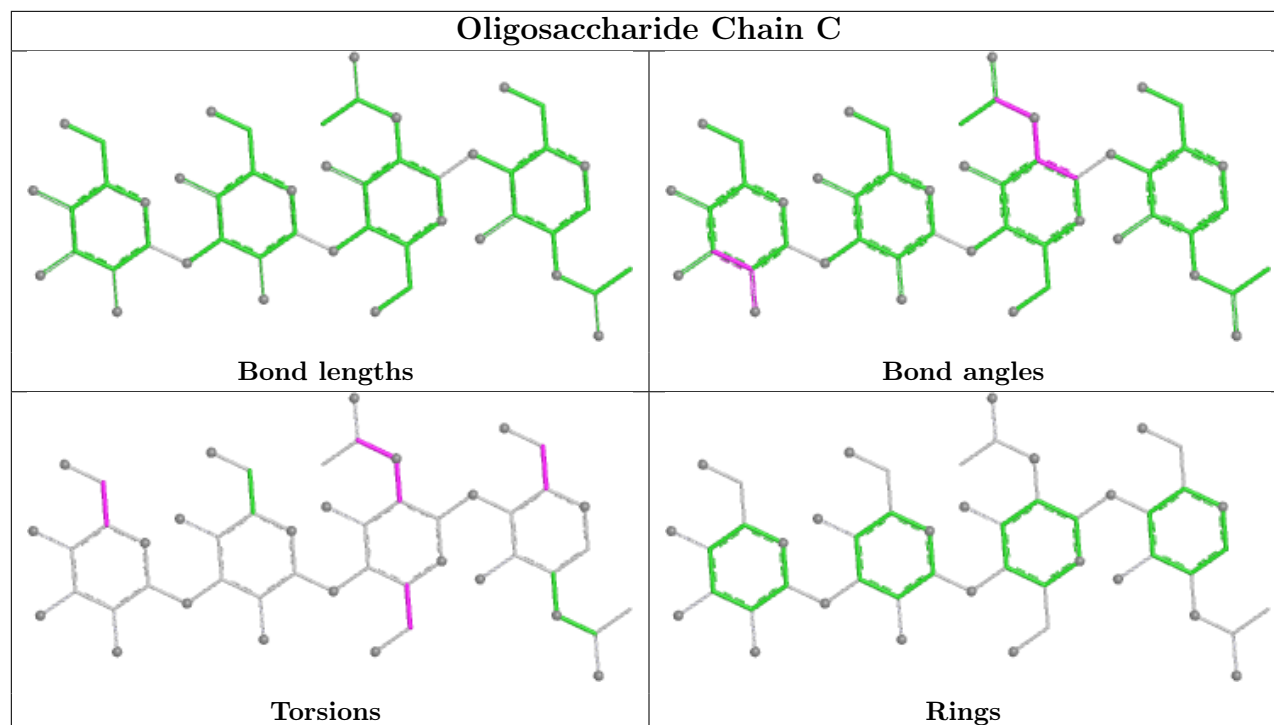
Mol	Chain	Res	Type	Atoms
2	E	4	MAN	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	D	3	BMA	O5-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	D	4	MAN	O5-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7
2	C	2	NAG	C3-C2-N2-C7

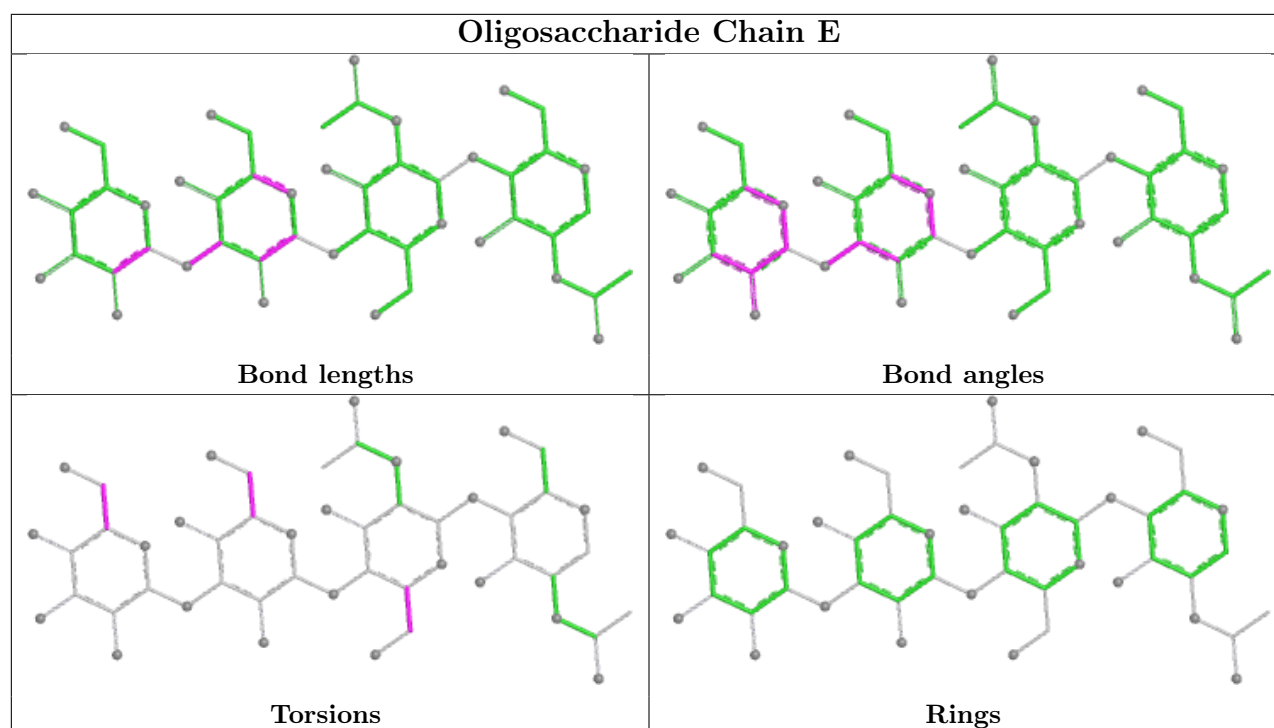
There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	3	BMA	2	0
2	C	1	NAG	1	0
2	C	3	BMA	1	0
2	E	4	MAN	2	0
2	C	2	NAG	2	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$
3	MAN	A	801	1	11,11,12	2.07	3 (27%)	15,15,17	2.73	3 (20%)
3	MAN	B	603	1	11,11,12	0.67	0	15,15,17	1.28	3 (20%)
3	MAN	B	604	1	11,11,12	0.94	1 (9%)	15,15,17	1.23	1 (6%)
3	MAN	B	605	1	11,11,12	0.70	0	15,15,17	1.74	4 (26%)
3	MAN	A	804	1	11,11,12	0.90	1 (9%)	15,15,17	0.94	1 (6%)
7	EDO	A	820	-	3,3,3	0.42	0	2,2,2	0.36	0
7	EDO	A	819	-	3,3,3	0.41	0	2,2,2	0.37	0
6	SO4	A	817	-	4,4,4	0.23	0	6,6,6	0.07	0
7	EDO	B	619	-	3,3,3	0.70	0	2,2,2	2.05	1 (50%)
3	MAN	B	602	1	11,11,12	0.66	0	15,15,17	1.20	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	A	802	1	11,11,12	0.84	0	15,15,17	1.48	2 (13%)
3	MAN	A	803	1	11,11,12	0.91	0	15,15,17	1.03	1 (6%)
4	NAG	A	805	1	14,14,15	1.08	2 (14%)	17,19,21	1.03	1 (5%)
7	EDO	B	618	-	3,3,3	0.41	0	2,2,2	0.34	0
4	NAG	B	601	1	14,14,15	0.52	0	17,19,21	0.67	1 (5%)
6	SO4	B	617	-	4,4,4	0.24	0	6,6,6	0.09	0
7	EDO	A	818	-	3,3,3	0.41	0	2,2,2	0.48	0
4	NAG	A	806	1	14,14,15	1.63	1 (7%)	17,19,21	1.63	4 (23%)

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	MAN	A	801	1	-	0/2/19/22	0/1/1/1
3	MAN	B	603	1	-	0/2/19/22	1/1/1/1
3	MAN	B	604	1	-	1/2/19/22	0/1/1/1
3	MAN	B	605	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	820	-	-	0/1/1/1	-
7	EDO	A	819	-	-	1/1/1/1	-
7	EDO	B	619	-	-	0/1/1/1	-
3	MAN	B	602	1	-	0/2/19/22	0/1/1/1
3	MAN	A	802	1	-	0/2/19/22	1/1/1/1
3	MAN	A	803	1	-	0/2/19/22	0/1/1/1
4	NAG	A	805	1	-	1/6/23/26	0/1/1/1
7	EDO	B	618	-	-	1/1/1/1	-
4	NAG	B	601	1	-	2/6/23/26	0/1/1/1
7	EDO	A	818	-	-	1/1/1/1	-
4	NAG	A	806	1	-	5/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	806	NAG	O5-C1	5.84	1.53	1.43
3	A	801	MAN	O6-C6	5.60	1.65	1.42
4	A	805	NAG	O5-C1	3.14	1.49	1.43
3	B	604	MAN	O5-C5	2.54	1.48	1.43
4	A	805	NAG	C1-C2	2.48	1.55	1.52
3	A	801	MAN	O5-C1	-2.35	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	MAN	O5-C5	2.14	1.47	1.43
3	A	804	MAN	O5-C1	-2.01	1.40	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	MAN	C1-O5-C5	9.48	124.89	112.19
3	B	605	MAN	C1-O5-C5	4.69	118.48	112.19
3	A	802	MAN	C1-O5-C5	4.59	118.33	112.19
4	A	806	NAG	C2-N2-C7	3.85	128.06	122.90
3	B	604	MAN	C1-O5-C5	3.68	117.12	112.19
3	B	603	MAN	C1-O5-C5	3.50	116.87	112.19
4	A	806	NAG	C1-O5-C5	3.48	116.85	112.19
4	A	805	NAG	C1-O5-C5	3.35	116.68	112.19
3	B	602	MAN	C1-O5-C5	3.35	116.67	112.19
3	B	605	MAN	O5-C1-C2	2.82	117.52	110.79
4	A	806	NAG	C1-C2-N2	2.74	114.75	110.43
3	A	803	MAN	C1-O5-C5	2.53	115.57	112.19
3	A	801	MAN	O5-C1-C2	2.42	116.56	110.79
4	B	601	NAG	C1-O5-C5	2.41	115.42	112.19
3	B	605	MAN	C1-C2-C3	2.37	113.10	109.64
3	A	802	MAN	O2-C2-C3	-2.35	105.28	110.15
7	B	619	EDO	O2-C2-C1	-2.24	95.32	112.39
3	B	602	MAN	O2-C2-C3	-2.22	105.55	110.15
4	A	806	NAG	C4-C3-C2	-2.20	107.79	111.02
3	B	605	MAN	O2-C2-C3	-2.16	105.67	110.15
3	B	603	MAN	O2-C2-C1	2.15	114.14	109.22
3	B	603	MAN	O2-C2-C3	-2.13	105.73	110.15
3	A	804	MAN	O2-C2-C3	-2.06	105.88	110.15
3	A	801	MAN	O2-C2-C3	-2.02	105.96	110.15

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	NAG	O5-C5-C6-O6
4	A	806	NAG	C8-C7-N2-C2
4	A	806	NAG	O7-C7-N2-C2
4	B	601	NAG	C4-C5-C6-O6
4	A	806	NAG	O5-C5-C6-O6
7	B	618	EDO	O1-C1-C2-O2
4	A	805	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	A	806	NAG	C1-C2-N2-C7
7	A	818	EDO	O1-C1-C2-O2
3	A	804	MAN	C4-C5-C6-O6
4	A	806	NAG	C3-C2-N2-C7
3	B	604	MAN	C4-C5-C6-O6
7	A	819	EDO	O1-C1-C2-O2

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	MAN	C1-C2-C3-C4-C5-O5
3	B	603	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
3	B	603	MAN	2	0
7	B	619	EDO	1	0
3	B	602	MAN	1	0
4	A	806	NAG	1	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%)	0.55	48 (10%) 11 9	67, 98, 216, 241	0
1	B	438/451 (97%)	0.17	12 (2%) 56 53	66, 92, 136, 180	0
All	All	881/902 (97%)	0.36	60 (6%) 23 20	66, 95, 205, 241	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	441	PHE	4.6
1	A	528	SER	4.1
1	A	513	VAL	4.0
1	A	543	THR	3.9
1	A	442	ILE	3.7
1	A	459	ILE	3.7
1	A	511	TYR	3.6
1	B	543	THR	3.5
1	A	432	LEU	3.4
1	A	498	ALA	3.3
1	A	527	THR	3.3
1	A	460	VAL	3.3
1	A	512	VAL	3.2
1	B	544	HIS	3.2
1	A	492	ALA	3.2
1	A	515	ILE	3.2
1	A	479	SER	3.1
1	A	517	VAL	2.9
1	A	526	VAL	2.9
1	A	457	ALA	2.9
1	A	507	PRO	2.8
1	A	481	THR	2.8
1	A	505	ASP	2.8
1	A	456	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	475	PHE	2.8
1	A	484	VAL	2.7
1	B	317	ALA	2.6
1	B	281	VAL	2.6
1	A	508	PHE	2.5
1	B	207	ILE	2.4
1	A	154	PRO	2.4
1	B	186	LEU	2.4
1	B	542	CYS	2.4
1	B	149	ILE	2.3
1	B	310	ARG	2.3
1	A	500	LEU	2.3
1	A	509	GLY	2.3
1	A	412	ILE	2.2
1	A	448	ILE	2.2
1	A	504	ASN	2.2
1	A	532	THR	2.2
1	A	447	VAL	2.2
1	A	488	TRP	2.2
1	A	107	ILE	2.2
1	A	462	VAL	2.2
1	B	536	CYS	2.1
1	A	392	ILE	2.1
1	A	155	PRO	2.1
1	A	452	PRO	2.1
1	A	477	LEU	2.1
1	A	529	LEU	2.1
1	A	160	PHE	2.1
1	A	313	SER	2.1
1	A	449	ILE	2.1
1	A	487	MET	2.0
1	B	127	VAL	2.0
1	A	530	ASP	2.0
1	A	522	GLY	2.0
1	B	150	ILE	2.0
1	A	351	VAL	2.0

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

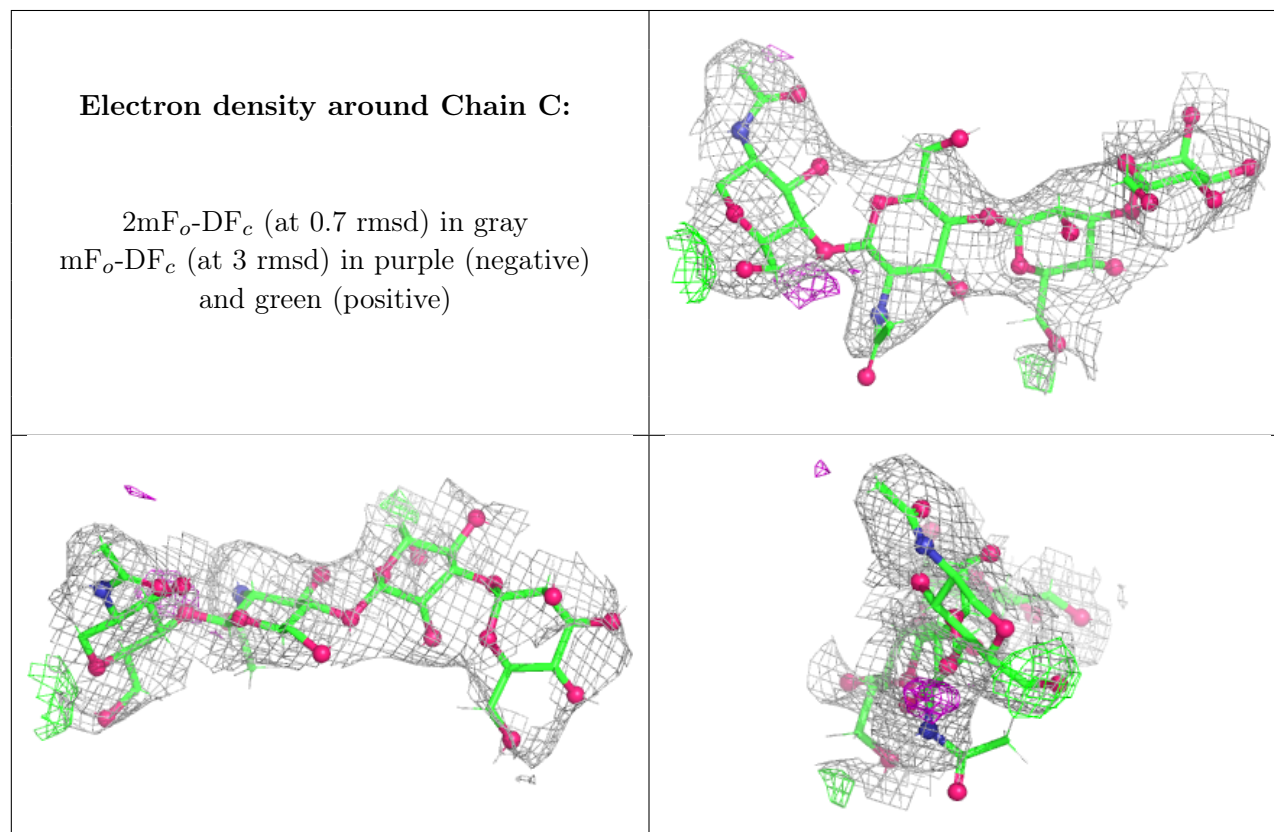
There are no non-standard protein/DNA/RNA residues in this entry.

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.

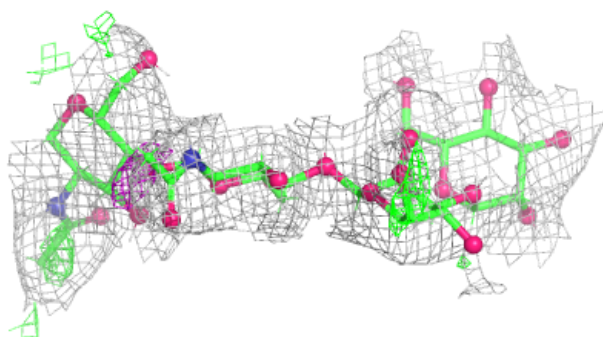
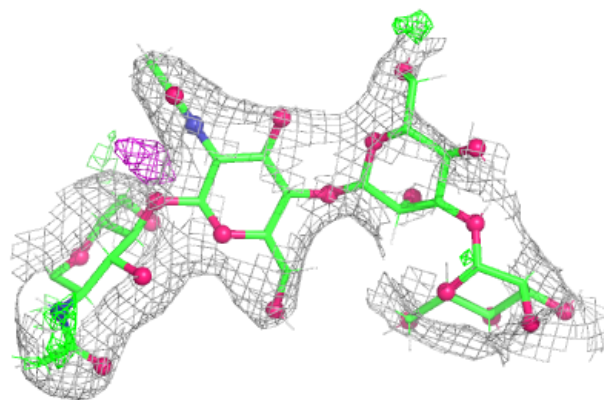
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	E	3	11/12	0.31	0.13	158,185,213,222	0
2	MAN	E	4	11/12	0.34	0.11	164,186,218,222	0
2	BMA	C	3	11/12	0.41	0.12	177,195,231,234	0
2	MAN	C	4	11/12	0.42	0.11	181,206,242,247	0
2	BMA	D	3	11/12	0.49	0.13	145,170,196,200	0
2	MAN	D	4	11/12	0.61	0.11	150,172,202,207	0
2	NAG	C	2	14/15	0.71	0.15	138,166,193,202	0
2	NAG	C	1	14/15	0.77	0.13	94,124,152,159	0
2	NAG	D	1	14/15	0.79	0.14	82,117,141,157	0
2	NAG	D	2	14/15	0.87	0.10	96,124,161,193	0
2	NAG	E	2	14/15	0.88	0.10	93,130,163,184	0
2	NAG	E	1	14/15	0.91	0.10	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.

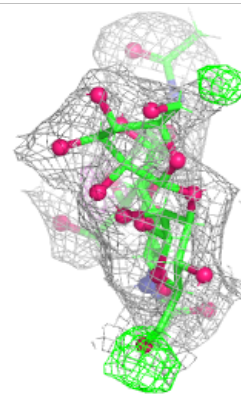
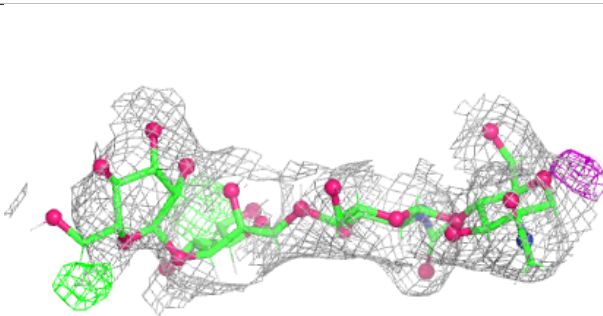
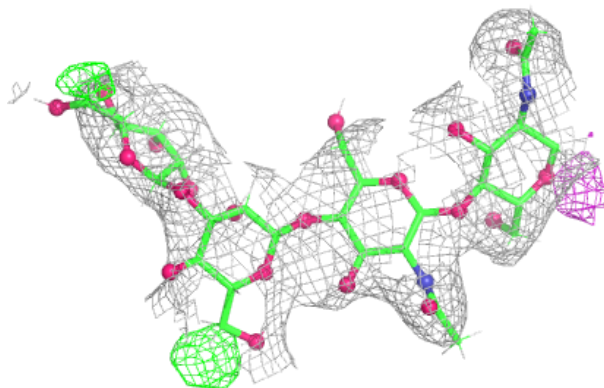


Electron density around Chain D:

$2mF_o-DF_c$ (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
7	EDO	A	820	4/4	0.46	0.19	98,118,122,133	0
3	MAN	B	603	11/12	0.53	0.14	124,149,179,185	0
3	MAN	B	605	11/12	0.60	0.12	124,149,178,179	0
7	EDO	A	819	4/4	0.62	0.15	135,162,168,168	0
4	NAG	A	806	14/15	0.65	0.10	164,197,226,234	0
3	MAN	B	602	11/12	0.66	0.12	117,146,169,179	0
3	MAN	A	801	11/12	0.66	0.16	114,136,159,176	0
3	MAN	A	804	11/12	0.67	0.12	113,147,171,194	0
4	NAG	A	805	14/15	0.70	0.13	121,149,181,193	0
3	MAN	B	604	11/12	0.74	0.14	116,143,183,187	0
7	EDO	A	818	4/4	0.76	0.29	106,128,132,132	0
3	MAN	A	803	11/12	0.79	0.11	94,119,141,144	0
3	MAN	A	802	11/12	0.80	0.11	108,133,157,166	0
7	EDO	B	619	4/4	0.80	0.20	97,132,142,158	0
6	SO4	A	817	5/5	0.81	0.07	150,154,165,171	0
4	NAG	B	601	14/15	0.82	0.12	99,123,145,155	0
7	EDO	B	618	4/4	0.84	0.10	92,110,126,126	0
6	SO4	B	617	5/5	0.84	0.10	139,141,148,165	0
5	CA	B	613	1/1	0.85	0.21	217,217,217,217	0
5	CA	B	616	1/1	0.91	0.14	119,119,119,119	0
5	CA	A	816	1/1	0.95	0.11	123,123,123,123	0
5	CA	B	606	1/1	0.97	0.09	103,103,103,103	0
5	CA	B	608	1/1	0.97	0.05	91,91,91,91	0
5	CA	A	810	1/1	0.97	0.11	83,83,83,83	0
5	CA	B	615	1/1	0.97	0.16	102,102,102,102	0
5	CA	A	813	1/1	0.98	0.10	119,119,119,119	0
5	CA	B	611	1/1	0.98	0.07	77,77,77,77	0
5	CA	A	814	1/1	0.98	0.11	110,110,110,110	0
5	CA	A	811	1/1	0.99	0.07	72,72,72,72	0
5	CA	A	812	1/1	0.99	0.04	74,74,74,74	0
5	CA	B	607	1/1	0.99	0.04	81,81,81,81	0
5	CA	A	809	1/1	0.99	0.07	76,76,76,76	0
5	CA	B	610	1/1	0.99	0.05	72,72,72,72	0
5	CA	A	807	1/1	0.99	0.14	116,116,116,116	0
5	CA	B	612	1/1	0.99	0.07	92,92,92,92	0
5	CA	A	815	1/1	0.99	0.07	86,86,86,86	0
5	CA	B	614	1/1	0.99	0.08	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	A	808	1/1	1.00	0.09	81,81,81,81	0
5	CA	B	609	1/1	1.00	0.02	75,75,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.