



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 28, 2024 – 09:05 AM EDT

PDB ID : 6VG1
Title : xenopus protocadherin 8.1 EC1-6
Authors : Harrison, O.J.; Brasch, B.; Shapiro, L.S.
Deposited on : 2020-01-07
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

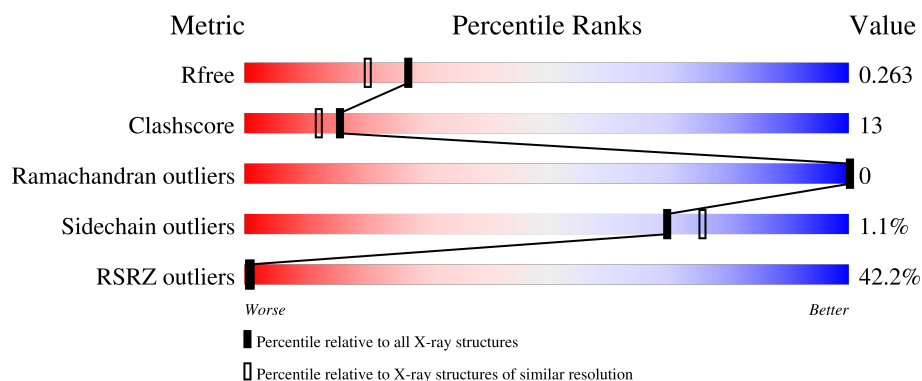
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	647	<div> <div>34%</div> <div>74%</div> <div>25%</div> </div>
1	B	647	<div> <div>50%</div> <div>72%</div> <div>27%</div> </div>
2	C	4	<div> <div>25%</div> <div>25%</div> <div>50%</div> </div>
2	D	4	<div> <div>50%</div> <div>25%</div> <div>25%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19847 atoms, of which 9678 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.

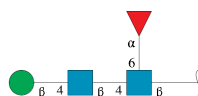
- Molecule 1 is a protein called protocadherin protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	642	Total	C	H	N	O	S	0	0	0
			9697	3078	4771	838	997	13			
1	B	641	Total	C	H	N	O	S	0	0	0
			9691	3075	4770	837	996	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	642	HIS	-	expression tag	UNP Q6GLU2
A	643	HIS	-	expression tag	UNP Q6GLU2
A	644	HIS	-	expression tag	UNP Q6GLU2
A	645	HIS	-	expression tag	UNP Q6GLU2
A	646	HIS	-	expression tag	UNP Q6GLU2
A	647	HIS	-	expression tag	UNP Q6GLU2
B	642	HIS	-	expression tag	UNP Q6GLU2
B	643	HIS	-	expression tag	UNP Q6GLU2
B	644	HIS	-	expression tag	UNP Q6GLU2
B	645	HIS	-	expression tag	UNP Q6GLU2
B	646	HIS	-	expression tag	UNP Q6GLU2
B	647	HIS	-	expression tag	UNP Q6GLU2

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



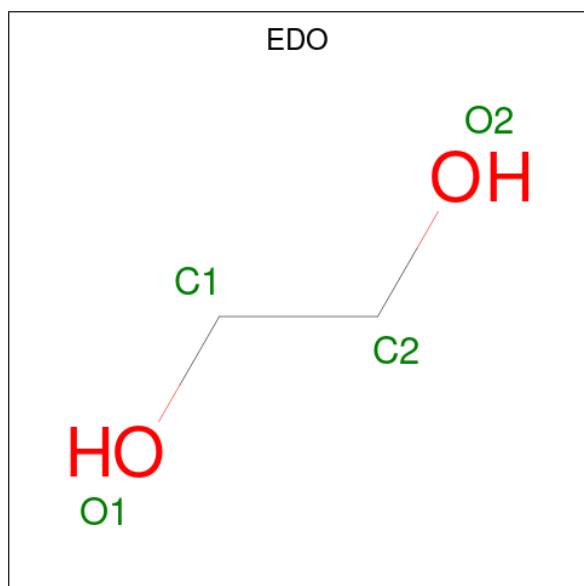
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	4	Total	C	H	N	O		0	0	0
			92	28	43	2	19				

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	4	Total	C	H	N	O	0	0	0
			92	28	43	2	19			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

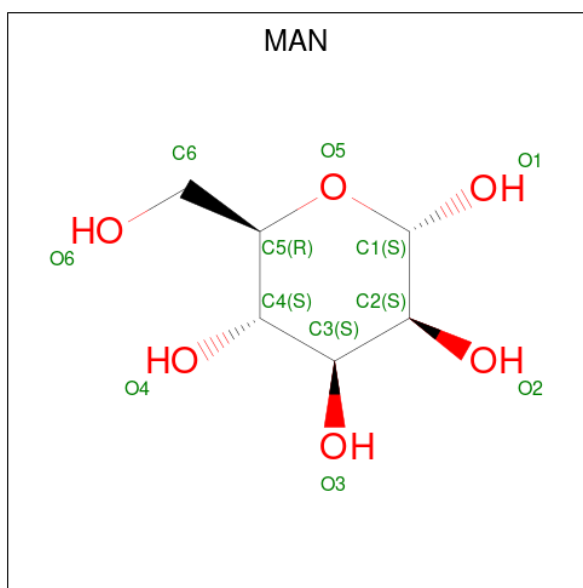
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	Ca	0	0
			15	15		
4	B	15	Total	Ca	0	0
			15	15		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			21	6	10	5		
6	A	1	Total	C	H	O	0	0
			21	6	10	5		
6	B	1	Total	C	H	O	0	0
			20	6	9	5		
6	B	1	Total	C	H	O	0	0
			21	6	10	5		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Na	0	0
			1	1		
7	B	1	Total	Na	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	81	Total	O	0	0
			81	81		
8	B	57	Total	O	0	0
			57	57		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	146.65Å 42.39Å 167.47Å 90.00° 110.60° 90.00°	Depositor
Resolution (Å)	38.27 – 2.00 38.27 – 2.00	Depositor EDS
% Data completeness (in resolution range)	45.0 (38.27-2.00) 41.9 (38.27-2.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.253 , 0.297 0.256 , 0.263	Depositor DCC
R_{free} test set	1775 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	19847	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.6680e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: EDO, NAG, CL, MAN, FUC, NA, BMA, CA

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	0.34	0/5010	0.55	0/6823
1	B	0.32	0/5005	0.53	0/6816
All	All	0.33	0/10015	0.54	0/13639

There are no bond length outliers.

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	4926	4771	4831	119	0
1	B	4921	4770	4828	141	0
2	C	49	43	43	1	0
2	D	49	43	43	2	0
3	A	4	6	6	1	0
3	B	4	6	6	0	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	22	20	20	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	22	19	19	2	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	81	0	0	0	0
8	B	57	0	0	1	0
All	All	10169	9678	9796	260	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 260 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:B:572:ASP:OD2	1:B:578:ASN:O	1.73	1.06
1:B:574:ASP:OD2	1:B:578:ASN:OD1	1.84	0.94
1:A:567:HIS:HE1	1:A:599:THR:HG22	1.32	0.92
1:B:220:GLU:HB3	1:B:311:ILE:HD11	1.56	0.86
1:B:557:SER:O	1:B:608:VAL:HG21	1.76	0.84

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	640/647 (99%)	612 (96%)	28 (4%)	0	100	100
1	B	639/647 (99%)	615 (96%)	24 (4%)	0	100	100
All	All	1279/1294 (99%)	1227 (96%)	52 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	549/555 (99%)	543 (99%)	6 (1%)	70	76
1	B	549/555 (99%)	543 (99%)	6 (1%)	70	76
All	All	1098/1110 (99%)	1086 (99%)	12 (1%)	70	76

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	155	ARG
1	B	218	MET
1	B	521	LEU
1	B	297	LEU
1	A	237	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	368	HIS
1	B	444	ASN
1	B	506	GLN
1	A	147	HIS
1	A	277	GLN

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 [i](#)

8 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	2,1	14,14,15	0.63	0	17,19,21	0.91	1 (5%)
2	NAG	C	2	2	14,14,15	0.41	0	17,19,21	0.52	0
2	BMA	C	3	2	11,11,12	0.98	0	15,15,17	0.78	1 (6%)
2	FUC	C	4	2	10,10,11	2.25	2 (20%)	14,14,16	1.89	2 (14%)
2	NAG	D	1	2,1	14,14,15	0.38	0	17,19,21	0.59	0
2	NAG	D	2	2	14,14,15	0.52	0	17,19,21	0.52	0
2	BMA	D	3	2	11,11,12	0.86	1 (9%)	15,15,17	0.97	0
2	FUC	D	4	2	10,10,11	1.33	2 (20%)	14,14,16	2.01	2 (14%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	FUC	C2-C3	5.01	1.60	1.52
2	C	4	FUC	C1-C2	3.91	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	FUC	O3-C3	2.65	1.49	1.43
2	D	4	FUC	O2-C2	2.34	1.48	1.43
2	D	3	BMA	C1-C2	2.05	1.57	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	FUC	O2-C2-C1	5.76	122.41	109.22
2	D	4	FUC	C1-C2-C3	5.73	117.98	109.64
2	D	4	FUC	C2-C3-C4	3.44	116.91	110.86
2	C	4	FUC	O2-C2-C3	-2.69	104.58	110.15
2	C	1	NAG	C4-C3-C2	2.14	114.15	111.02

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

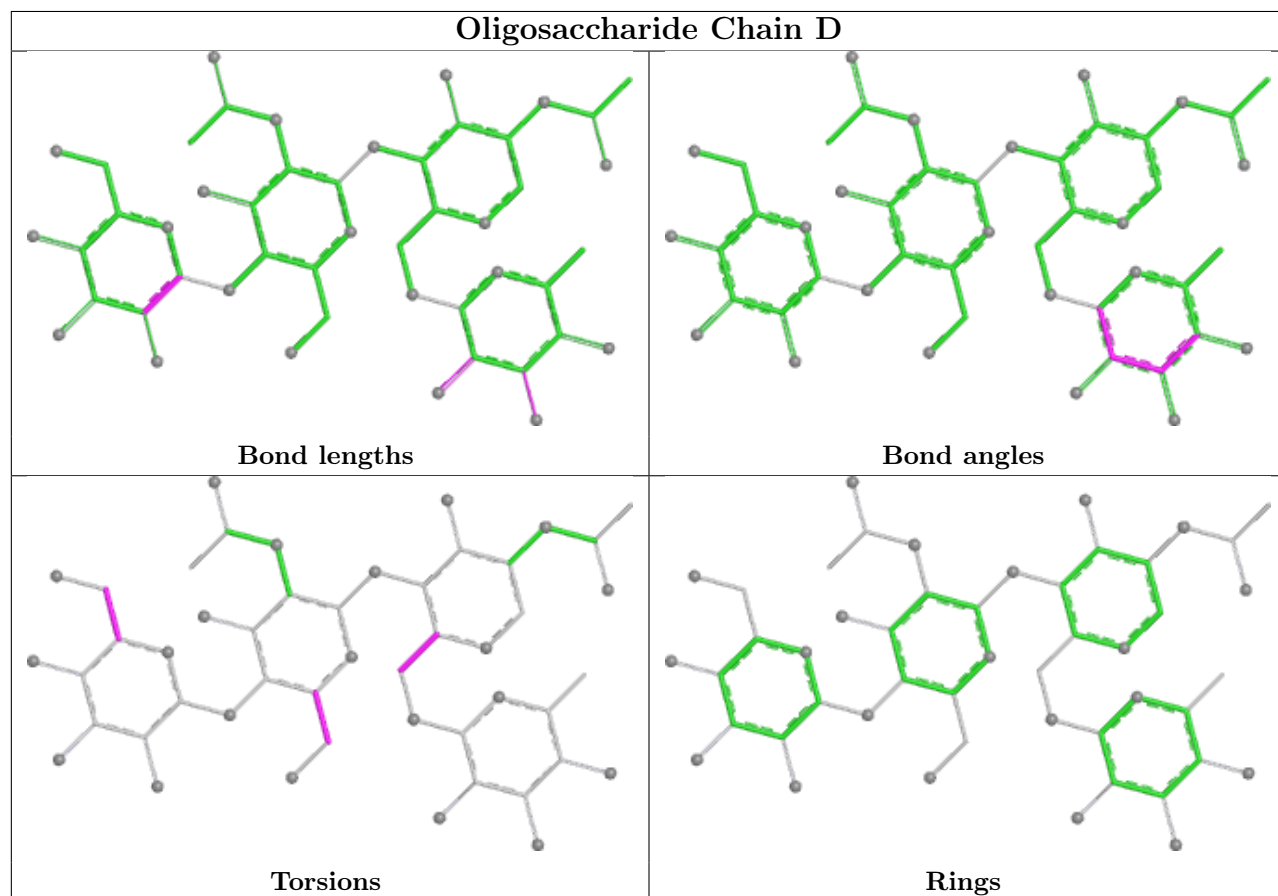
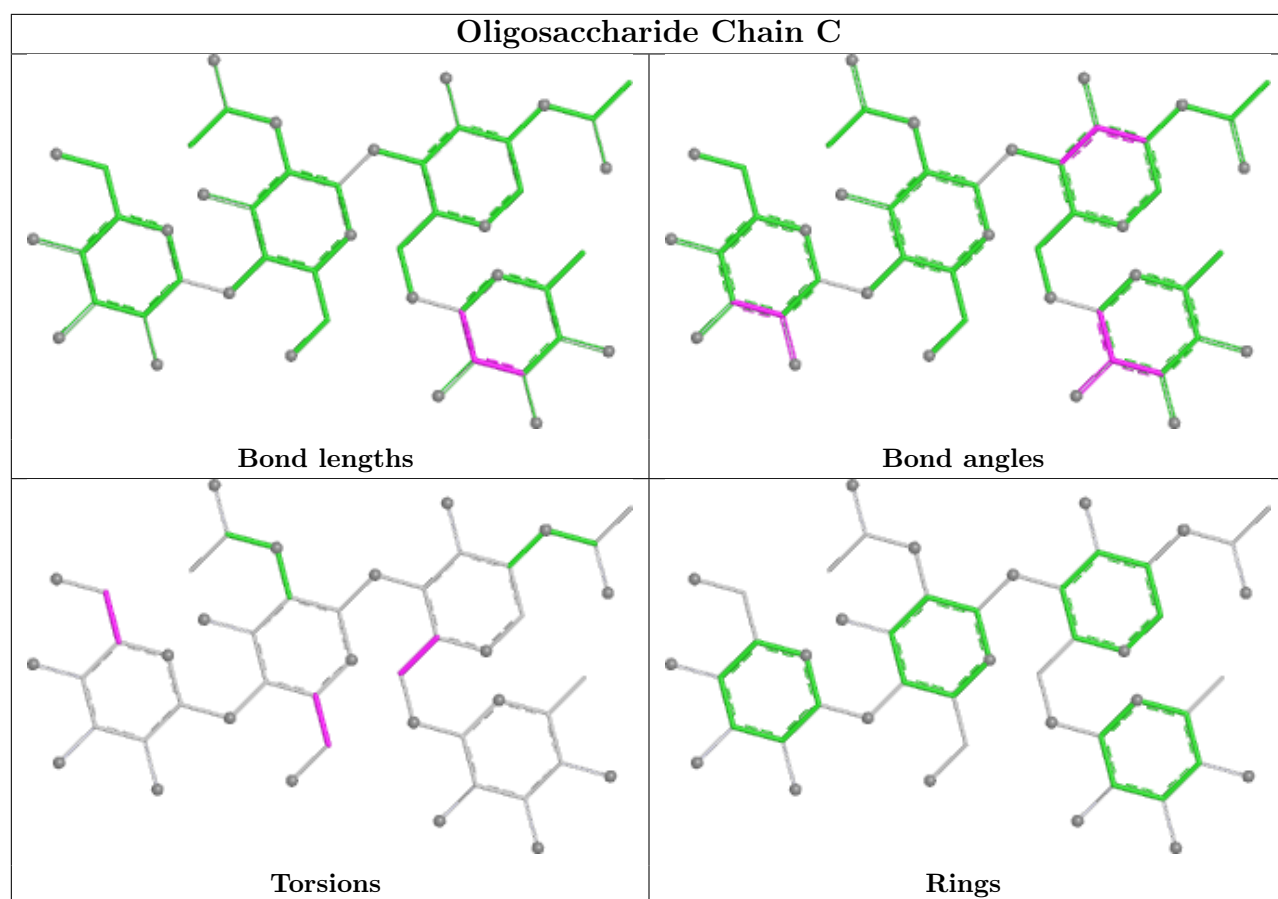
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
2	D	4	FUC	2	0
2	C	4	FUC	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

Of 40 ligands modelled in this entry, 34 are monoatomic - leaving 6 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	EDO	A	705	-	3,3,3	0.46	0	2,2,2	0.60	0
6	MAN	A	722	1	11,11,12	0.90	0	15,15,17	1.11	1 (6%)
3	EDO	B	724	-	3,3,3	0.46	0	2,2,2	0.49	0
6	MAN	B	722	1	11,11,12	1.27	1 (9%)	15,15,17	1.10	1 (6%)
6	MAN	A	723	1	11,11,12	1.01	0	15,15,17	1.35	3 (20%)
6	MAN	B	721	1	11,11,12	1.60	2 (18%)	15,15,17	1.32	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
3	EDO	A	705	-	-	0/1/1/1	-
6	MAN	A	722	1	-	0/2/19/22	0/1/1/1
3	EDO	B	724	-	-	1/1/1/1	-
6	MAN	B	722	1	-	0/2/19/22	0/1/1/1
6	MAN	A	723	1	-	2/2/19/22	0/1/1/1
6	MAN	B	721	1	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	721	MAN	O4-C4	3.13	1.50	1.43
6	B	721	MAN	O5-C1	-2.96	1.38	1.43
6	B	722	MAN	C2-C3	2.18	1.55	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	723	MAN	C1-O5-C5	3.48	116.85	112.19
6	A	722	MAN	C1-O5-C5	2.51	115.55	112.19
6	B	721	MAN	O2-C2-C3	-2.19	105.62	110.15
6	A	723	MAN	C2-C3-C4	2.19	114.71	110.86
6	A	723	MAN	O5-C5-C4	-2.14	105.63	110.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	723	MAN	O5-C5-C6-O6
6	A	723	MAN	C4-C5-C6-O6
6	B	721	MAN	O5-C5-C6-O6
3	B	724	EDO	O1-C1-C2-O2
6	B	721	MAN	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	705	EDO	1	0
6	B	722	MAN	2	0
6	A	723	MAN	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	642/647 (99%)	1.65	217 (33%) 1 1	12, 65, 130, 196	0
1	B	641/647 (99%)	2.32	324 (50%) 0 1	21, 81, 156, 231	0
All	All	1283/1294 (99%)	1.99	541 (42%) 1 1	12, 72, 145, 231	0

The worst 5 of 541 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	616	PHE	10.1
1	B	556	PRO	8.6
1	A	616	PHE	8.5
1	B	555	VAL	8.4
1	B	568	ILE	8.1

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	0.55	0.17	75,105,115,135	0
2	BMA	D	3	11/12	0.68	0.16	58,83,100,104	0
2	FUC	D	4	10/11	0.70	0.22	43,76,96,115	0
2	NAG	D	2	14/15	0.73	0.18	57,83,113,141	0
2	NAG	D	1	14/15	0.74	0.19	36,72,104,114	0

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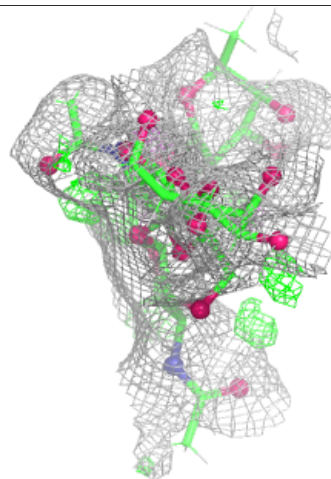
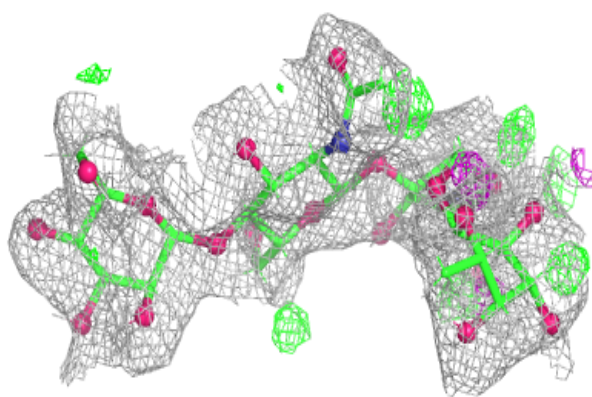
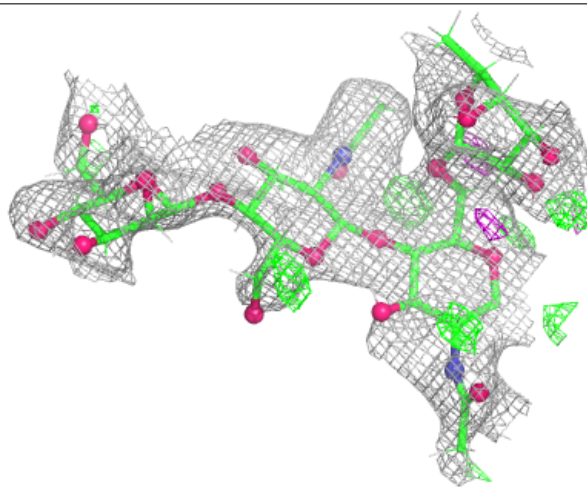
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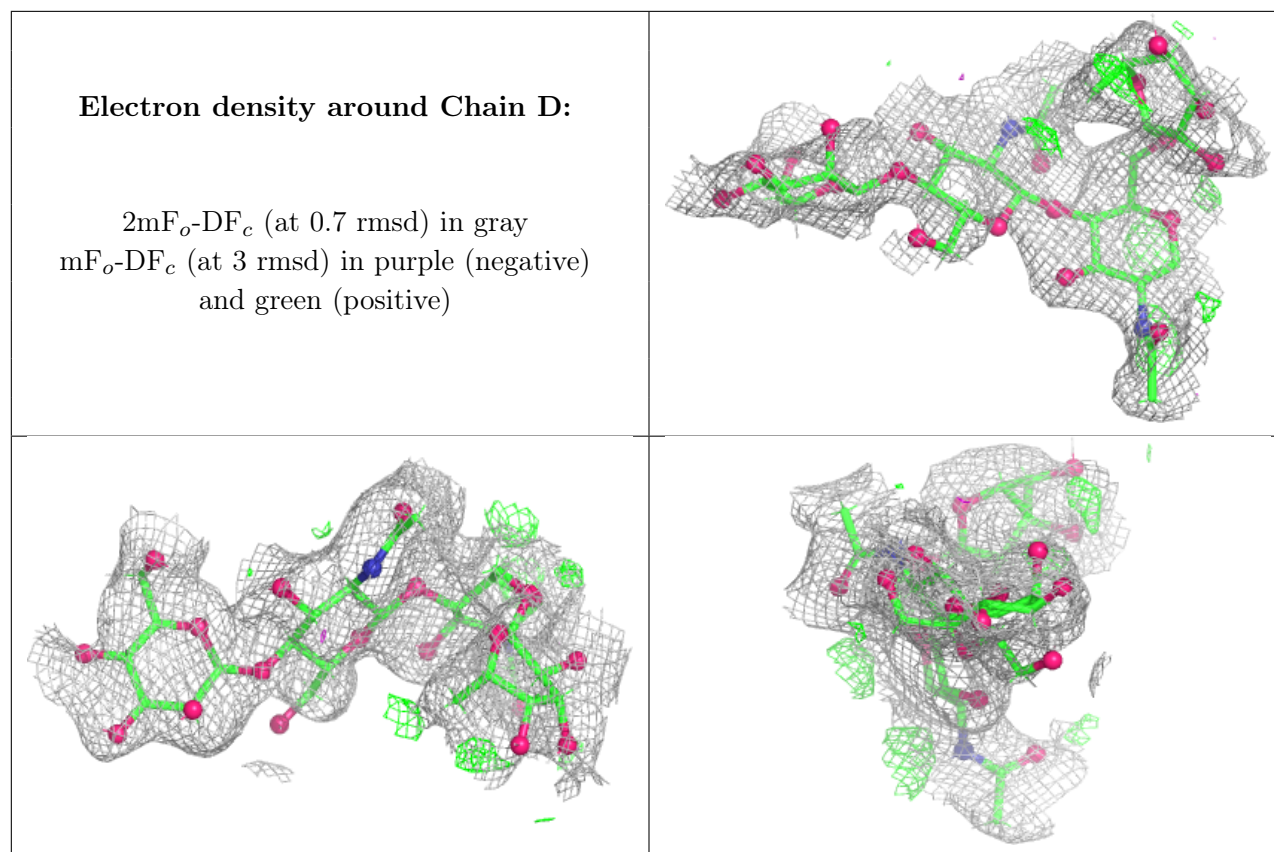
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	C	2	14/15	0.78	0.17	42,73,106,128	0
2	FUC	C	4	10/11	0.82	0.21	45,72,105,127	0
2	NAG	C	1	14/15	0.87	0.17	31,56,88,95	0

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 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, 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
6	MAN	B	722	11/12	0.52	0.26	64,110,135,158	0
6	MAN	B	721	11/12	0.60	0.19	66,94,131,142	0
6	MAN	A	722	11/12	0.67	0.18	49,82,99,109	0
6	MAN	A	723	11/12	0.69	0.22	56,81,104,132	0
4	CA	B	719	1/1	0.78	0.17	154,154,154,154	0
4	CA	B	706	1/1	0.86	0.12	92,92,92,92	0
3	EDO	B	724	4/4	0.86	0.17	42,65,79,88	0
4	CA	B	705	1/1	0.88	0.11	75,75,75,75	0
5	CL	B	720	1/1	0.88	0.25	69,69,69,69	0
4	CA	B	707	1/1	0.89	0.13	122,122,122,122	0
4	CA	B	714	1/1	0.90	0.11	62,62,62,62	0
5	CL	A	721	1/1	0.91	0.15	43,43,43,43	0
4	CA	B	708	1/1	0.91	0.12	74,74,74,74	0
3	EDO	A	705	4/4	0.93	0.14	25,57,69,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CA	B	718	1/1	0.94	0.10	88,88,88,88	0
4	CA	A	719	1/1	0.95	0.07	91,91,91,91	0
4	CA	B	712	1/1	0.95	0.16	52,52,52,52	0
4	CA	A	718	1/1	0.95	0.08	69,69,69,69	0
4	CA	B	717	1/1	0.95	0.09	83,83,83,83	0
7	NA	B	723	1/1	0.95	0.10	46,46,46,46	0
4	CA	A	707	1/1	0.96	0.08	58,58,58,58	0
4	CA	A	715	1/1	0.96	0.05	44,44,44,44	0
4	CA	B	710	1/1	0.97	0.04	32,32,32,32	0
4	CA	A	716	1/1	0.97	0.05	52,52,52,52	0
4	CA	B	713	1/1	0.97	0.08	38,38,38,38	0
4	CA	A	717	1/1	0.97	0.07	62,62,62,62	0
4	CA	B	715	1/1	0.97	0.05	44,44,44,44	0
4	CA	B	716	1/1	0.97	0.05	59,59,59,59	0
4	CA	A	714	1/1	0.97	0.09	29,29,29,29	0
4	CA	A	711	1/1	0.97	0.04	34,34,34,34	0
4	CA	A	709	1/1	0.98	0.04	21,21,21,21	0
4	CA	B	709	1/1	0.98	0.07	47,47,47,47	0
4	CA	A	720	1/1	0.98	0.05	48,48,48,48	0
4	CA	A	706	1/1	0.98	0.08	56,56,56,56	0
4	CA	A	712	1/1	0.98	0.05	33,33,33,33	0
4	CA	A	708	1/1	0.98	0.04	56,56,56,56	0
7	NA	A	724	1/1	0.99	0.02	14,14,14,14	0
4	CA	A	710	1/1	0.99	0.02	23,23,23,23	0
4	CA	A	713	1/1	1.00	0.01	18,18,18,18	0
4	CA	B	711	1/1	1.00	0.01	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.