



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2022 – 02:13 PM EDT

PDB ID : 5T9T
Title : Protocadherin Gamma B2 extracellular cadherin domains 1-5
Authors : Goodman, K.M.; Mannepalli, S.; Bahna, F.; Honig, B.; Shapiro, L.
Deposited on : 2016-09-09
Resolution : 3.50 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 : 2.27
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) : 2.27

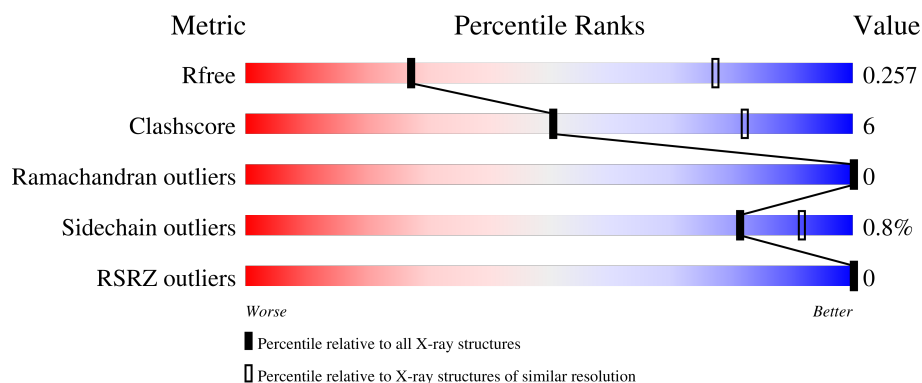
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	535	
1	B	535	
2	C	4	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8223 atoms, of which 0 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.

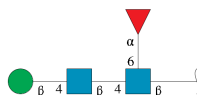
- Molecule 1 is a protein called Protocadherin gamma B2-alpha C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	526	Total	C	N	O	S	0	0	0
			4009	2503	682	817	7			
1	B	526	Total	C	N	O	S	0	0	0
			3972	2483	671	811	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	528	HIS	-	expression tag	UNP Q8K486
A	529	HIS	-	expression tag	UNP Q8K486
A	530	HIS	-	expression tag	UNP Q8K486
A	531	HIS	-	expression tag	UNP Q8K486
A	532	HIS	-	expression tag	UNP Q8K486
A	533	HIS	-	expression tag	UNP Q8K486
A	534	HIS	-	expression tag	UNP Q8K486
A	535	HIS	-	expression tag	UNP Q8K486
B	528	HIS	-	expression tag	UNP Q8K486
B	529	HIS	-	expression tag	UNP Q8K486
B	530	HIS	-	expression tag	UNP Q8K486
B	531	HIS	-	expression tag	UNP Q8K486
B	532	HIS	-	expression tag	UNP Q8K486
B	533	HIS	-	expression tag	UNP Q8K486
B	534	HIS	-	expression tag	UNP Q8K486
B	535	HIS	-	expression tag	UNP Q8K486

- 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.

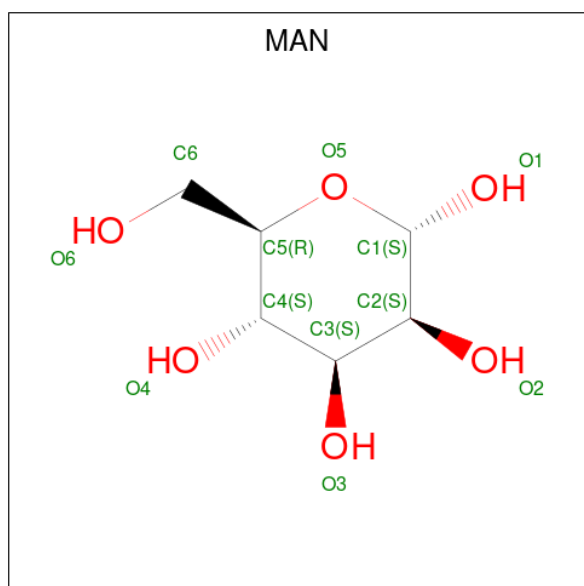


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	Ca	0	0
			12	12		
3	B	14	Total	Ca	0	0
			14	14		

- Molecule 4 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



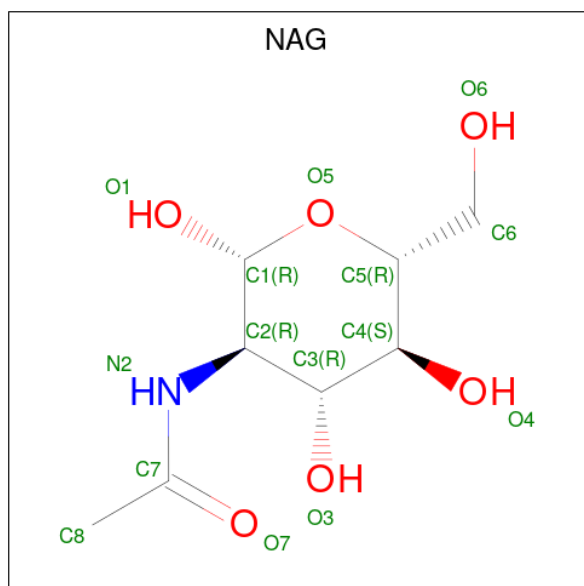
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

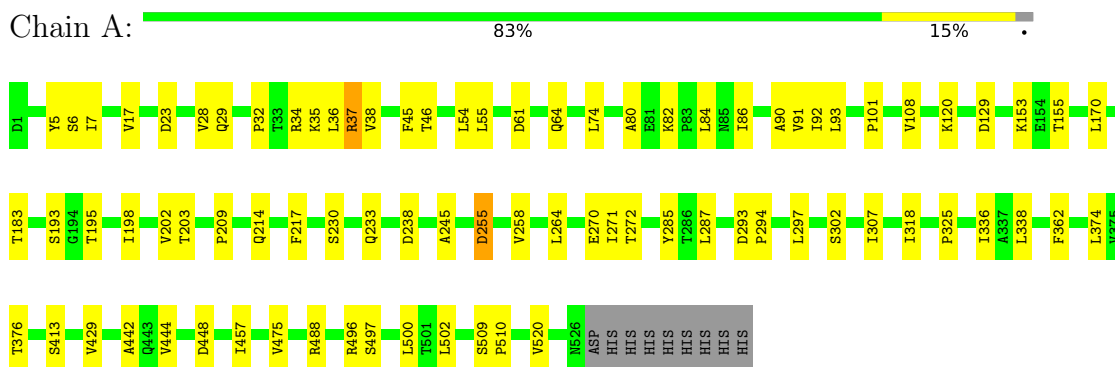
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	B	3	Total	O	0	0
			3	3		

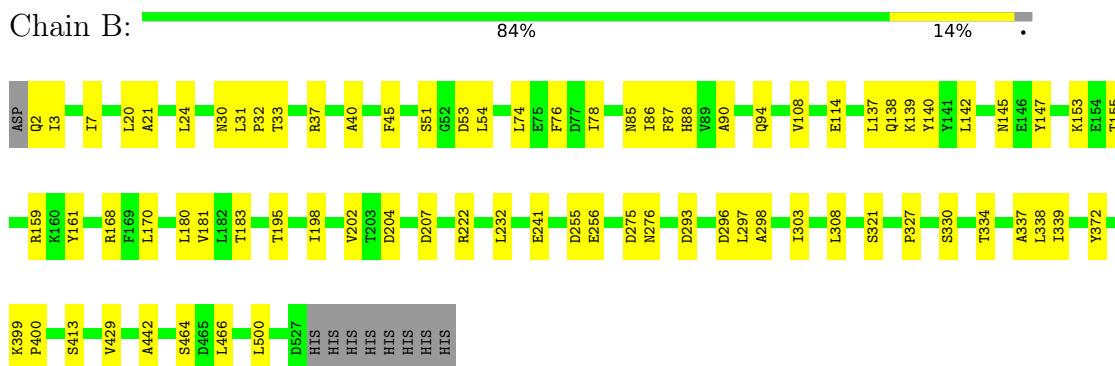
3 Residue-property plots

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: Protocadherin gamma B2-alpha C



• Molecule 1: Protocadherin gamma B2-alpha C



• Molecule 2: 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.72Å 118.07Å 98.19Å 90.00° 103.91° 90.00°	Depositor
Resolution (Å)	39.75 – 3.50 39.75 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.75-3.50) 86.8 (39.75-3.50)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.213 , 0.257 0.213 , 0.257	Depositor DCC
R_{free} test set	1088 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8223	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, FUC, MAN, 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	0.25	0/4084	0.46	0/5582
1	B	0.25	0/4048	0.47	0/5543
All	All	0.25	0/8132	0.47	0/11125

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 [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	4009	0	3821	48	0
1	B	3972	0	3740	47	0
2	C	49	0	43	0	0
3	A	12	0	0	0	0
3	B	14	0	0	0	0
4	A	55	0	50	1	0
4	B	66	0	60	0	0
5	A	28	0	26	0	0
5	B	14	0	13	0	0
6	A	1	0	0	0	0
6	B	3	0	0	0	0
All	All	8223	0	7753	91	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 6.

All (91) 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:74:LEU:O	1:A:90:ALA:HA	1.92	0.70
1:A:183:THR:HG22	1:A:195:THR:HG22	1.72	0.70
1:A:35:LYS:NZ	1:A:37:ARG:HE	1.91	0.68
1:A:238:ASP:OD2	1:A:245:ALA:HA	1.96	0.65
1:A:35:LYS:HZ3	1:A:37:ARG:HE	1.47	0.63
1:B:183:THR:HG22	1:B:195:THR:HG22	1.79	0.63
1:B:464:SER:HB3	1:B:500:LEU:HD12	1.83	0.60
1:A:429:VAL:HG11	1:A:442:ALA:HB2	1.84	0.59
1:A:5:TYR:HB2	1:A:91:VAL:HG12	1.86	0.57
1:A:230:SER:HA	1:A:272:THR:HG22	1.86	0.57
1:B:139:LYS:NZ	1:B:140:TYR:O	2.37	0.57
1:A:233:GLN:HA	1:A:270:GLU:HA	1.86	0.57
1:A:475:VAL:HG21	1:A:500:LEU:HD11	1.88	0.55
1:B:147:TYR:HE1	1:B:168:ARG:HH11	1.55	0.55
1:B:30:ASN:O	1:B:33:THR:HG22	2.08	0.54
1:A:336:ILE:HD11	1:A:376:THR:HG22	1.91	0.52
1:A:120:LYS:NZ	1:B:298:ALA:O	2.42	0.52
1:A:293:ASP:HB2	1:A:294:PRO:HD2	1.92	0.52
1:B:21:ALA:HB1	1:B:31:LEU:HD11	1.93	0.51
1:A:448:ASP:HB2	1:A:457:ILE:HD11	1.93	0.51
1:B:275:ASP:OD2	1:B:276:ASN:N	2.35	0.51
1:B:170:LEU:HD13	1:B:202:VAL:HG22	1.92	0.51
1:A:497:SER:HA	1:A:520:VAL:O	2.10	0.51
1:A:5:TYR:OH	1:A:23:ASP:OD2	2.24	0.50
1:A:46:THR:O	1:A:55:LEU:HB2	2.12	0.50
1:A:209:PRO:HB3	1:A:297:LEU:HB3	1.94	0.50
1:A:264:LEU:HD12	1:A:271:ILE:HG12	1.93	0.50
1:B:232:LEU:HD23	1:B:303:ILE:HD13	1.93	0.50
1:A:325:PRO:HB2	1:A:413:SER:HB3	1.94	0.49
1:B:85:ASN:OD1	1:B:86:ILE:N	2.38	0.49
1:B:74:LEU:O	1:B:90:ALA:HA	2.13	0.49
1:B:3:ILE:HD11	1:B:24:LEU:HD23	1.95	0.49
1:B:145:ASN:HD21	1:B:180:LEU:HD21	1.78	0.49
1:B:429:VAL:HG21	1:B:442:ALA:HB2	1.95	0.48
1:A:101:PRO:HB3	1:A:129:ASP:HB2	1.94	0.48
1:A:285:TYR:HE2	1:A:307:ILE:HD11	1.79	0.48
1:A:61:ASP:HB3	1:A:64:GLN:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:VAL:O	1:A:32:PRO:HD3	2.14	0.47
1:B:147:TYR:CE1	1:B:168:ARG:HD3	2.49	0.47
1:A:6:SER:HA	1:A:92:ILE:O	2.15	0.47
1:B:114:GLU:OE2	1:B:207:ASP:OD2	2.33	0.47
1:A:108:VAL:HG13	1:A:198:ILE:HG23	1.97	0.46
1:B:45:PHE:HB3	1:B:54:LEU:HD11	1.97	0.46
1:A:36:LEU:HD23	1:A:36:LEU:HA	1.79	0.46
1:A:35:LYS:O	1:A:80:ALA:HA	2.15	0.46
1:B:137:LEU:O	1:B:138:GLN:NE2	2.48	0.46
1:A:444:VAL:HG11	1:A:502:LEU:HD22	1.97	0.46
1:B:7:ILE:O	1:B:94:GLN:HG2	2.15	0.46
1:A:362:PHE:HB3	1:A:374:LEU:HD11	1.97	0.46
1:A:86:ILE:HB	1:B:338:LEU:HD23	1.98	0.45
1:B:37:ARG:O	1:B:78:ILE:HA	2.16	0.45
1:B:466:LEU:HD12	1:B:466:LEU:H	1.81	0.45
1:A:170:LEU:HD13	1:A:202:VAL:HG22	1.97	0.45
1:A:7:ILE:O	1:A:93:LEU:HA	2.16	0.45
1:B:155:THR:HG21	1:B:159:ARG:HH21	1.81	0.45
1:B:108:VAL:HG23	1:B:198:ILE:HG23	1.98	0.45
1:B:330:SER:HB3	1:B:334:THR:HG21	1.99	0.45
1:B:327:PRO:HA	1:B:413:SER:HB3	1.99	0.45
1:B:222:ARG:HA	1:B:308:LEU:HB2	1.99	0.45
1:A:214:GLN:HB2	1:A:217:PHE:CE1	2.52	0.44
1:B:51:SER:OG	1:B:53:ASP:OD1	2.34	0.44
1:A:82:LYS:HA	1:A:82:LYS:HD3	1.91	0.44
1:B:31:LEU:N	1:B:32:PRO:HD2	2.32	0.44
1:B:204:ASP:OD2	1:B:241:GLU:N	2.43	0.44
1:A:287:LEU:O	1:A:302:SER:HA	2.18	0.44
1:A:509:SER:HA	1:A:510:PRO:HA	1.78	0.44
1:B:24:LEU:HD22	1:B:87:PHE:CD1	2.53	0.44
1:A:17:VAL:HB	1:A:54:LEU:HB3	2.00	0.44
1:A:193:SER:HB2	4:A:613:MAN:H2	1.59	0.44
1:A:153:LYS:HE2	1:A:155:THR:HG22	1.99	0.43
1:A:38:VAL:HG21	1:A:45:PHE:O	2.19	0.43
1:B:399:LYS:HA	1:B:400:PRO:HA	1.87	0.43
1:B:155:THR:HG21	1:B:159:ARG:HE	1.85	0.42
1:B:54:LEU:HD21	1:B:76:PHE:HZ	1.85	0.42
1:B:293:ASP:OD2	1:B:297:LEU:HD12	2.20	0.42
1:B:147:TYR:HE1	1:B:168:ARG:HD3	1.83	0.42
1:B:153:LYS:HD3	1:B:161:TYR:OH	2.19	0.42
1:A:29:GLN:O	1:A:32:PRO:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ILE:HD13	1:A:318:ILE:HA	1.94	0.42
1:B:2:GLN:HA	1:B:88:HIS:O	2.19	0.42
1:B:255:ASP:OD1	1:B:256:GLU:N	2.53	0.42
1:A:255:ASP:N	1:A:255:ASP:OD1	2.52	0.42
1:A:255:ASP:HB2	1:A:258:VAL:HG23	2.01	0.42
1:B:40:ALA:HB2	1:B:76:PHE:HB2	2.01	0.42
1:B:142:LEU:HD12	1:B:181:VAL:O	2.20	0.42
1:B:139:LYS:HD2	1:B:140:TYR:H	1.85	0.41
1:B:321:SER:O	1:B:337:ALA:HA	2.21	0.41
1:A:203:THR:OG1	1:B:296:ASP:OD2	2.27	0.41
1:A:35:LYS:HB3	1:A:35:LYS:HE3	1.77	0.41
1:A:84:LEU:HD23	1:B:338:LEU:HD13	2.02	0.40
1:B:339:ILE:HB	1:B:372:TYR:HB2	2.03	0.40

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	524/535 (98%)	505 (96%)	19 (4%)	0	100	100
1	B	524/535 (98%)	503 (96%)	21 (4%)	0	100	100
All	All	1048/1070 (98%)	1008 (96%)	40 (4%)	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	447/476 (94%)	441 (99%)	6 (1%)	69	86
1	B	438/476 (92%)	437 (100%)	1 (0%)	93	98
All	All	885/952 (93%)	878 (99%)	7 (1%)	81	91

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ARG
1	A	37	ARG
1	A	255	ASP
1	A	338	LEU
1	A	488	ARG
1	A	496	ARG
1	B	20	LEU

Sometimes 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 ⓘ

4 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	0.22	0	17,19,21	0.54	0
2	NAG	C	2	2	14,14,15	0.27	0	17,19,21	0.46	0
2	BMA	C	3	2	11,11,12	0.71	0	15,15,17	0.79	0
2	FUC	C	4	2	10,10,11	0.88	0	14,14,16	0.99	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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	FUC	C	4	2	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

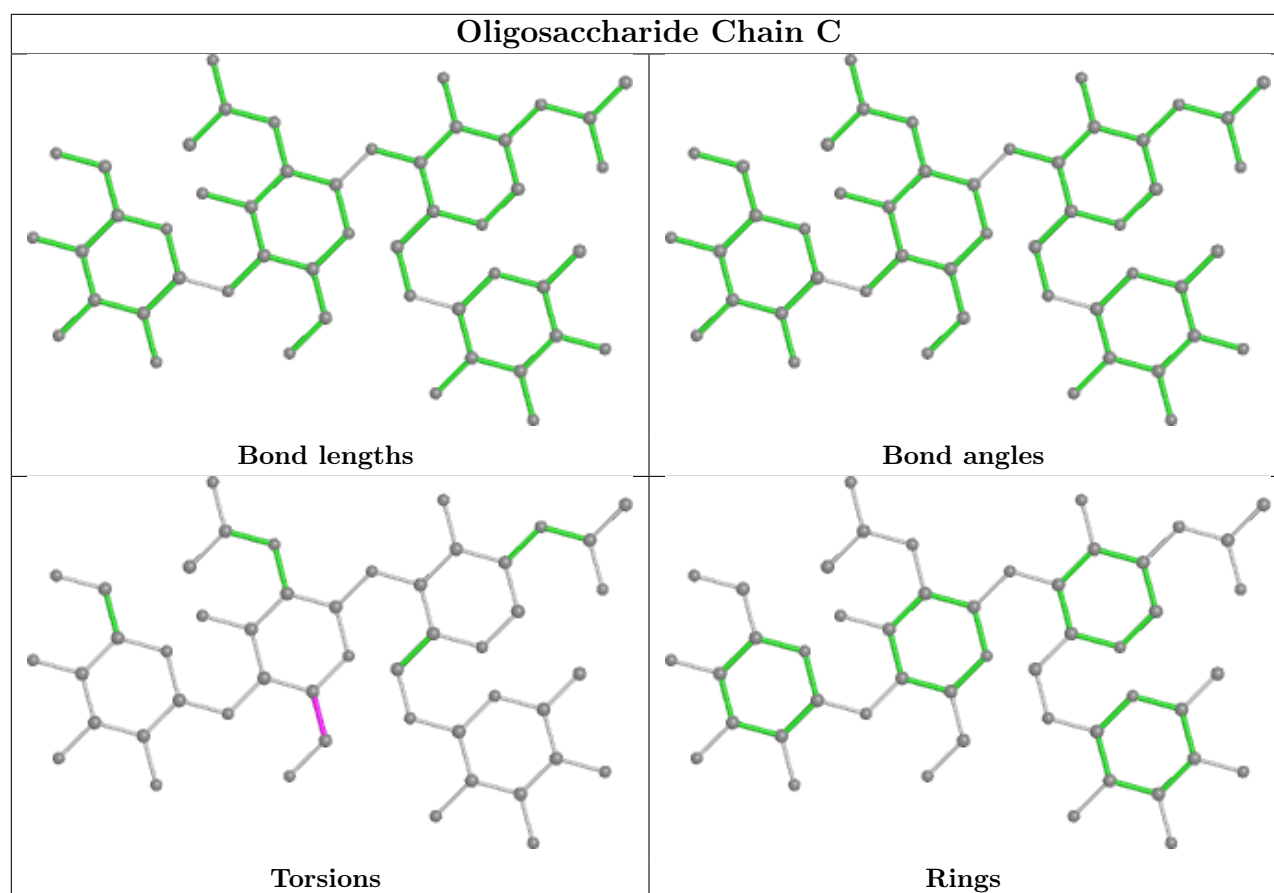
All (2) torsion outliers are listed below:

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

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](#)

Of 40 ligands modelled in this entry, 26 are monoatomic - leaving 14 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	MAN	B	624	1	11,11,12	0.79	0	15,15,17	0.91	0
4	MAN	A	616	1	11,11,12	0.62	0	15,15,17	1.15	2 (13%)
4	MAN	A	614	1	11,11,12	0.75	0	15,15,17	1.18	2 (13%)
5	NAG	B	625	1	14,14,15	0.42	0	17,19,21	0.56	0
4	MAN	B	616	1	11,11,12	0.71	0	15,15,17	1.08	2 (13%)
4	MAN	B	623	1	11,11,12	0.71	0	15,15,17	1.24	2 (13%)
4	MAN	B	617	1	11,11,12	0.80	0	15,15,17	1.18	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	617	1	14,14,15	0.21	0	17,19,21	0.55	0
4	MAN	A	619	1	11,11,12	0.85	0	15,15,17	0.85	1 (6%)
4	MAN	A	618	1	11,11,12	0.54	0	15,15,17	1.43	3 (20%)
4	MAN	B	615	1	11,11,12	0.71	0	15,15,17	0.98	2 (13%)
5	NAG	A	615	1	14,14,15	0.35	0	17,19,21	0.47	0
4	MAN	A	613	1	11,11,12	0.87	0	15,15,17	0.97	1 (6%)
4	MAN	B	622	1	11,11,12	0.75	0	15,15,17	1.08	2 (13%)

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	MAN	B	624	1	-	0/2/19/22	0/1/1/1
4	MAN	A	616	1	-	2/2/19/22	0/1/1/1
4	MAN	A	614	1	-	0/2/19/22	0/1/1/1
5	NAG	B	625	1	-	2/6/23/26	0/1/1/1
4	MAN	B	616	1	-	0/2/19/22	0/1/1/1
4	MAN	B	623	1	-	0/2/19/22	0/1/1/1
4	MAN	B	617	1	-	0/2/19/22	0/1/1/1
5	NAG	A	617	1	-	1/6/23/26	0/1/1/1
4	MAN	A	619	1	-	0/2/19/22	0/1/1/1
4	MAN	A	618	1	-	0/2/19/22	0/1/1/1
4	MAN	B	615	1	-	0/2/19/22	0/1/1/1
5	NAG	A	615	1	-	0/6/23/26	0/1/1/1
4	MAN	A	613	1	-	0/2/19/22	0/1/1/1
4	MAN	B	622	1	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	618	MAN	C1-O5-C5	3.83	117.39	112.19
4	B	623	MAN	C1-O5-C5	3.16	116.48	112.19
4	A	614	MAN	C1-O5-C5	2.95	116.19	112.19
4	A	616	MAN	C1-O5-C5	2.84	116.05	112.19
4	B	617	MAN	C1-O5-C5	2.75	115.91	112.19
4	A	618	MAN	O5-C1-C2	2.58	114.76	110.77
4	B	616	MAN	C1-O5-C5	2.58	115.68	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	615	MAN	C1-O5-C5	2.50	115.58	112.19
4	B	622	MAN	C1-O5-C5	2.40	115.45	112.19
4	B	623	MAN	O2-C2-C3	-2.28	105.57	110.14
4	A	618	MAN	O2-C2-C3	-2.27	105.59	110.14
4	B	622	MAN	O2-C2-C3	-2.26	105.62	110.14
4	B	616	MAN	O2-C2-C3	-2.17	105.80	110.14
4	A	616	MAN	O2-C2-C3	-2.15	105.83	110.14
4	B	617	MAN	O2-C2-C3	-2.13	105.88	110.14
4	B	615	MAN	O2-C2-C3	-2.13	105.88	110.14
4	A	619	MAN	O2-C2-C3	-2.13	105.88	110.14
4	A	614	MAN	O2-C2-C3	-2.11	105.91	110.14
4	A	613	MAN	O2-C2-C3	-2.05	106.03	110.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	616	MAN	C4-C5-C6-O6
5	B	625	NAG	O5-C5-C6-O6
4	A	616	MAN	O5-C5-C6-O6
5	B	625	NAG	C4-C5-C6-O6
5	A	617	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	613	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	526/535 (98%)	-0.48	0 100 100	38, 75, 122, 160	0
1	B	526/535 (98%)	-0.47	0 100 100	42, 73, 110, 148	0
All	All	1052/1070 (98%)	-0.47	0 100 100	38, 74, 118, 160	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

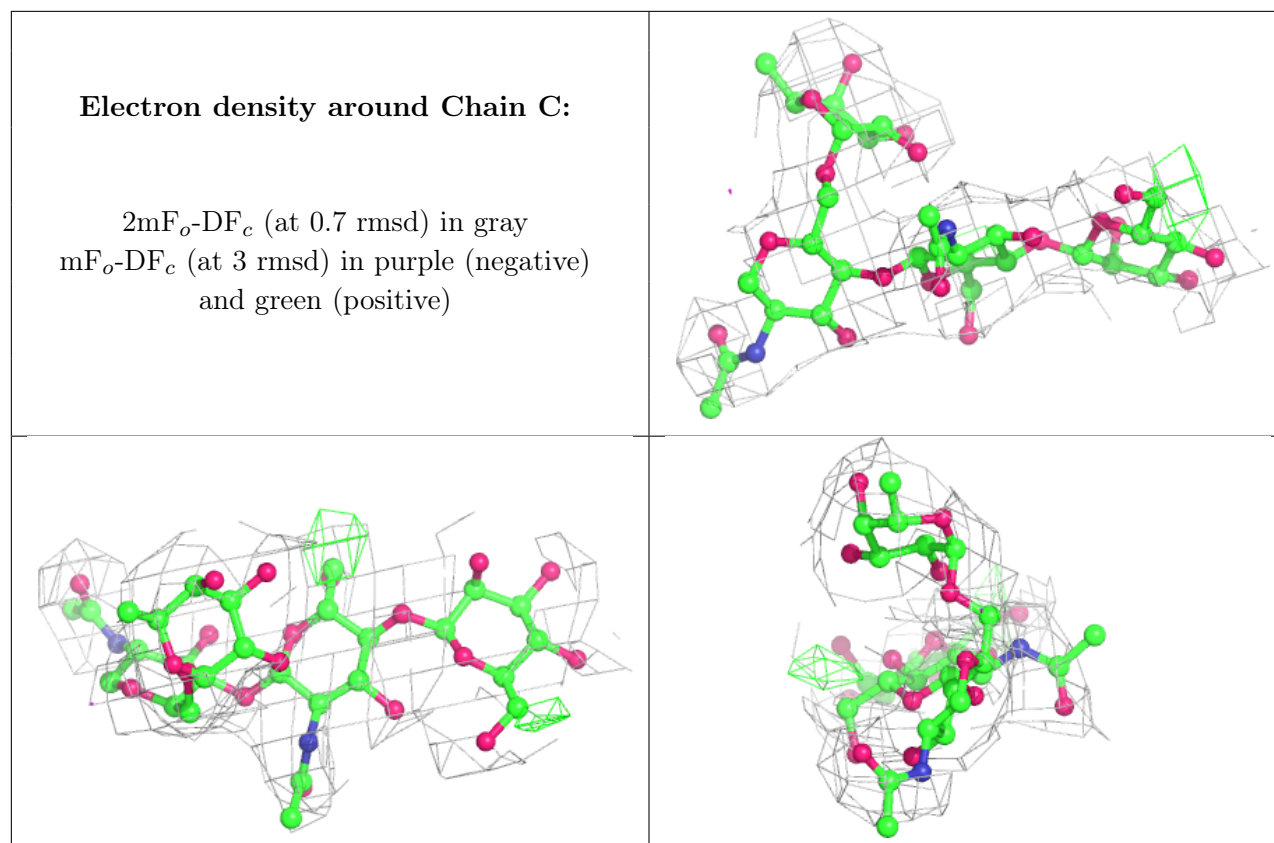
There are no non-standard protein/DNA/RNA residues in this entry.

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	0.81	0.17	103,117,123,128	0
2	FUC	C	4	10/11	0.87	0.21	90,95,107,110	0
2	NAG	C	2	14/15	0.89	0.23	110,116,122,125	0
2	NAG	C	1	14/15	0.91	0.21	80,92,112,113	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.



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
4	MAN	A	619	11/12	0.78	0.36	110,121,126,127	0
5	NAG	B	625	14/15	0.78	0.18	69,85,90,91	0
5	NAG	A	615	14/15	0.82	0.21	80,90,101,102	0
4	MAN	B	622	11/12	0.82	0.32	99,106,115,117	0
4	MAN	B	615	11/12	0.83	0.32	74,87,106,114	0
3	CA	A	606	1/1	0.86	0.10	45,45,45,45	0
4	MAN	B	617	11/12	0.87	0.18	81,95,110,112	0
5	NAG	A	617	14/15	0.87	0.29	107,121,133,140	0
4	MAN	A	613	11/12	0.87	0.24	92,101,105,108	0
3	CA	A	602	1/1	0.88	0.12	89,89,89,89	0
4	MAN	A	618	11/12	0.88	0.35	106,117,126,133	0
3	CA	B	604	1/1	0.88	0.15	69,69,69,69	0
4	MAN	A	614	11/12	0.89	0.19	70,80,94,99	0
3	CA	B	613	1/1	0.89	0.08	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MAN	B	624	11/12	0.89	0.28	84,94,97,100	0
3	CA	B	610	1/1	0.90	0.22	59,59,59,59	0
4	MAN	B	623	11/12	0.90	0.23	90,98,106,113	0
4	MAN	A	616	11/12	0.90	0.24	94,111,128,132	0
4	MAN	B	616	11/12	0.93	0.18	74,87,94,99	0
3	CA	A	612	1/1	0.94	0.07	50,50,50,50	0
3	CA	A	605	1/1	0.94	0.09	40,40,40,40	0
3	CA	A	611	1/1	0.94	0.14	50,50,50,50	0
3	CA	B	607	1/1	0.95	0.11	51,51,51,51	0
3	CA	B	601	1/1	0.95	0.07	48,48,48,48	0
3	CA	B	612	1/1	0.95	0.12	38,38,38,38	0
3	CA	A	608	1/1	0.95	0.10	46,46,46,46	0
3	CA	B	605	1/1	0.95	0.11	33,33,33,33	0
3	CA	B	606	1/1	0.95	0.08	51,51,51,51	0
3	CA	A	601	1/1	0.96	0.13	66,66,66,66	0
3	CA	A	607	1/1	0.96	0.14	56,56,56,56	0
3	CA	B	602	1/1	0.96	0.04	29,29,29,29	0
3	CA	A	610	1/1	0.97	0.12	43,43,43,43	0
3	CA	A	604	1/1	0.97	0.11	62,62,62,62	0
3	CA	B	611	1/1	0.98	0.16	45,45,45,45	0
3	CA	B	603	1/1	0.98	0.11	63,63,63,63	0
3	CA	B	608	1/1	0.98	0.07	42,42,42,42	0
3	CA	B	614	1/1	0.98	0.16	166,166,166,166	0
3	CA	B	609	1/1	0.98	0.10	52,52,52,52	0
3	CA	A	603	1/1	0.98	0.04	74,74,74,74	0
3	CA	A	609	1/1	0.99	0.10	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.