



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 11:04 AM EDT

PDB ID : 6EET  
Title : Crystal structure of mouse Protocadherin-15 EC9-MAD12  
Authors : Narui, Y.; Sotomayor, M.  
Deposited on : 2018-08-15  
Resolution : 3.23 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

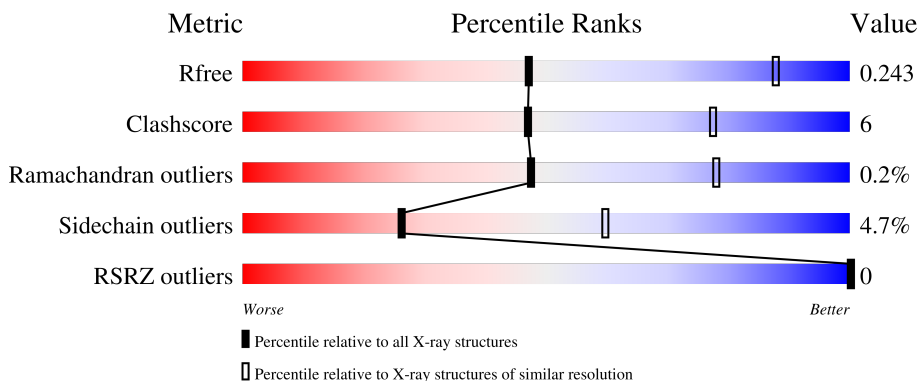
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.23 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	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	474	 75% 18% 7%
2	B	2	 100%
2	C	2	 100%

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 3584 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-15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	443	3476	2211	583	673	9	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

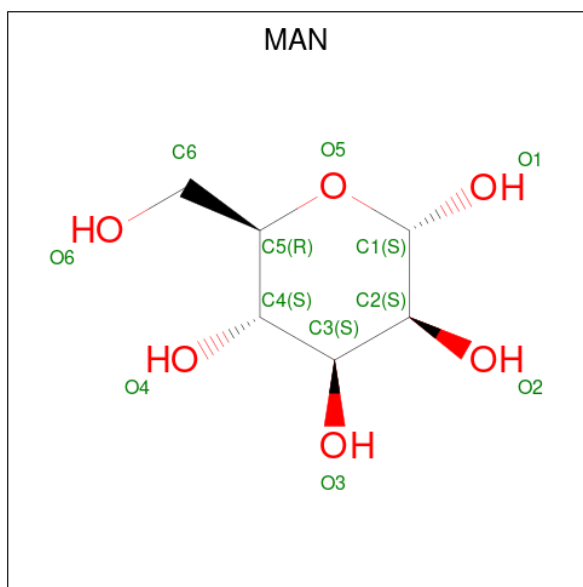
Chain	Residue	Modelled	Actual	Comment	Reference
A	1354	LYS	-	expression tag	UNP Q99PJ1
A	1355	VAL	-	expression tag	UNP Q99PJ1
A	1356	PRO	-	expression tag	UNP Q99PJ1
A	1357	ARG	-	expression tag	UNP Q99PJ1
A	1358	ALA	-	expression tag	UNP Q99PJ1
A	1359	ARG	-	expression tag	UNP Q99PJ1
A	1360	ASP	-	expression tag	UNP Q99PJ1
A	1361	PRO	-	expression tag	UNP Q99PJ1
A	1362	PRO	-	expression tag	UNP Q99PJ1
A	1363	VAL	-	expression tag	UNP Q99PJ1
A	1364	GLY	-	expression tag	UNP Q99PJ1
A	1365	GLY	-	expression tag	UNP Q99PJ1
A	1366	HIS	-	expression tag	UNP Q99PJ1
A	1367	HIS	-	expression tag	UNP Q99PJ1
A	1368	HIS	-	expression tag	UNP Q99PJ1
A	1369	HIS	-	expression tag	UNP Q99PJ1
A	1370	HIS	-	expression tag	UNP Q99PJ1
A	1371	HIS	-	expression tag	UNP Q99PJ1

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	15	8	2	4	1	0	0

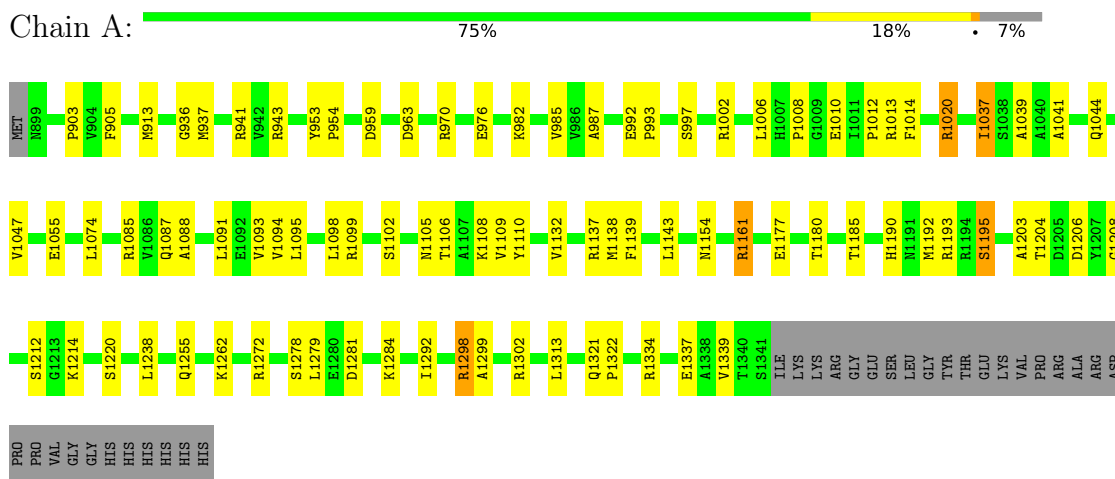
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	4	4	4	0	0

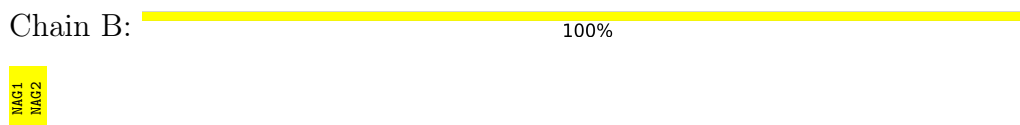
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Protocadherin-15



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucofuranose



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucofuranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.51Å 170.06Å 91.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.81 – 3.23 45.76 – 3.23	Depositor EDS
% Data completeness (in resolution range)	99.2 (45.81-3.23) 99.3 (45.76-3.23)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 3.25Å)	Xtrriage
Refinement program	REFMAC 5.8.0230	Depositor
R, $R_{free}$	0.176 , 0.234 0.182 , 0.243	Depositor DCC
$R_{free}$ test set	790 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	97.2	Xtrriage
Anisotropy	0.345	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 58.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3584	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, NAG, 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	0.43	0/3547	0.69	0/4825

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1020	ARG	Sidechain
1	A	1137	ARG	Sidechain
1	A	1161	ARG	Sidechain
1	A	1193	ARG	Sidechain
1	A	1272	ARG	Sidechain
1	A	943	ARG	Sidechain

### 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	3476	0	3462	43	0
2	B	28	0	25	0	0
2	C	28	0	25	0	0
3	A	33	0	30	1	0
4	A	15	0	18	0	0
5	A	4	0	0	0	0
All	All	3584	0	3560	44	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 (44) 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:1192:MET:O	1:A:1195:SER:HB2	1.81	0.80
1:A:959:ASP:OD2	1:A:970:ARG:NH1	2.28	0.67
3:A:1405:MAN:H2	3:A:1408:MAN:O3	1.97	0.64
1:A:1085:ARG:HH21	1:A:1108:LYS:CE	2.11	0.62
1:A:1012:PRO:HA	1:A:1041:ALA:HB2	1.82	0.62
1:A:1094:VAL:HG23	1:A:1099:ARG:NH2	2.15	0.61
1:A:1321:GLN:OE1	1:A:1321:GLN:HA	2.03	0.58
1:A:1093:VAL:HG12	1:A:1098:LEU:O	2.04	0.56
1:A:1085:ARG:HH21	1:A:1108:LYS:HE2	1.71	0.55
1:A:1020:ARG:NH1	1:A:1110:TYR:CD2	2.75	0.54
1:A:1020:ARG:NH1	1:A:1110:TYR:CE2	2.76	0.54
1:A:913:MET:HB3	1:A:1006:LEU:HD21	1.89	0.53
1:A:905:PHE:CZ	1:A:987:ALA:HB2	2.44	0.53
1:A:1010:GLU:O	1:A:1044:GLN:NE2	2.42	0.53
1:A:1085:ARG:HH21	1:A:1108:LYS:HE3	1.75	0.50
1:A:1088:ALA:O	1:A:1105:ASN:HB2	2.12	0.49
1:A:1302:ARG:NH1	1:A:1339:VAL:HG11	2.28	0.49
1:A:1139:PHE:HA	1:A:1185:THR:O	2.13	0.48
1:A:1302:ARG:NH1	1:A:1339:VAL:HG21	2.28	0.48
1:A:905:PHE:CZ	1:A:985:VAL:HG23	2.48	0.48
1:A:1334:ARG:NH2	1:A:1337:GLU:OE1	2.36	0.47
1:A:1190:HIS:O	1:A:1192:MET:HG3	2.14	0.47
1:A:1091:LEU:O	1:A:1095:LEU:HG	2.15	0.46
1:A:1238:LEU:HD23	1:A:1238:LEU:O	2.16	0.46
1:A:1298:ARG:HH11	1:A:1298:ARG:HG3	1.81	0.46
1:A:1102:SER:N	1:A:1105:ASN:OD1	2.50	0.44
1:A:953:TYR:HB3	1:A:954:PRO:HD3	1.99	0.44
1:A:936:GLY:O	1:A:937:MET:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1154:ASN:O	1:A:1206:ASP:HA	2.19	0.43
1:A:1203:ALA:O	1:A:1212:SER:HA	2.19	0.43
1:A:992:GLU:HA	1:A:993:PRO:HA	1.92	0.43
1:A:982:LYS:HE2	1:A:1002:ARG:NH1	2.35	0.42
1:A:1087:GLN:HG3	1:A:1106:THR:HG22	2.01	0.42
1:A:1014:PHE:CD1	1:A:1039:ALA:HB2	2.54	0.41
1:A:903:PRO:O	1:A:997:SER:HB3	2.20	0.41
1:A:941:ARG:HH22	1:A:963:ASP:CG	2.24	0.41
1:A:1037:ILE:HD11	1:A:1109:VAL:HG22	2.01	0.41
1:A:1204:THR:HB	1:A:1208:GLY:HA2	2.02	0.41
1:A:1091:LEU:O	1:A:1094:VAL:HG12	2.21	0.41
1:A:1220:SER:HB3	1:A:1292:ILE:HD12	2.03	0.41
1:A:1281:ASP:OD2	1:A:1284:LYS:HG2	2.20	0.40
1:A:1321:GLN:N	1:A:1322:PRO:HD2	2.35	0.40
1:A:1177:GLU:HB2	1:A:1180:THR:OG1	2.21	0.40
1:A:1138:MET:O	1:A:1139:PHE:HB2	2.22	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	441/474 (93%)	411 (93%)	29 (7%)	1 (0%)	47 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1299	ALA

### 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	385/411 (94%)	367 (95%)	18 (5%)	26 60

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	976	GLU
1	A	1008	PRO
1	A	1013	ARG
1	A	1037	ILE
1	A	1047	VAL
1	A	1055	GLU
1	A	1074	LEU
1	A	1132	VAL
1	A	1143	LEU
1	A	1161	ARG
1	A	1195	SER
1	A	1214	LYS
1	A	1255	GLN
1	A	1262	LYS
1	A	1278	SER
1	A	1279	LEU
1	A	1298	ARG
1	A	1313	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	950	GLN
1	A	1087	GLN
1	A	1223	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

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	B	1	2,1	14,14,15	0.76	0	17,19,21	1.94	3 (17%)
2	NAG	B	2	2	14,14,15	0.68	0	17,19,21	1.42	4 (23%)
2	NAG	C	1	2,1	14,14,15	1.31	2 (14%)	17,19,21	2.90	9 (52%)
2	NAG	C	2	2	14,14,15	0.65	0	17,19,21	1.61	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
2	NAG	B	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	C6-C5	2.73	1.61	1.51
2	C	1	NAG	O5-C1	2.22	1.47	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-O5-C5	6.48	120.98	112.19
2	C	1	NAG	C1-O5-C5	6.07	120.41	112.19
2	C	1	NAG	O5-C5-C6	4.99	115.03	107.20
2	C	2	NAG	O5-C5-C6	4.40	114.11	107.20
2	C	1	NAG	O4-C4-C3	-4.26	100.51	110.35
2	C	1	NAG	C4-C3-C2	4.08	117.00	111.02
2	C	1	NAG	O6-C6-C5	3.63	123.75	111.29
2	B	2	NAG	C4-C3-C2	2.91	115.28	111.02
2	B	2	NAG	O5-C5-C6	2.80	111.60	107.20
2	C	1	NAG	O5-C1-C2	-2.65	107.10	111.29
2	C	1	NAG	C6-C5-C4	2.47	118.79	113.00
2	B	1	NAG	O5-C1-C2	-2.41	107.48	111.29
2	C	1	NAG	C1-C2-N2	-2.40	106.38	110.49
2	C	1	NAG	O4-C4-C5	2.34	115.11	109.30
2	C	2	NAG	O5-C1-C2	-2.32	107.63	111.29
2	B	2	NAG	C1-C2-N2	2.27	114.36	110.49
2	B	2	NAG	C2-N2-C7	2.25	126.10	122.90
2	C	2	NAG	C4-C3-C2	2.24	114.30	111.02
2	C	2	NAG	C6-C5-C4	-2.12	108.05	113.00
2	B	1	NAG	O5-C5-C4	2.04	115.79	110.83

There are no chirality outliers.

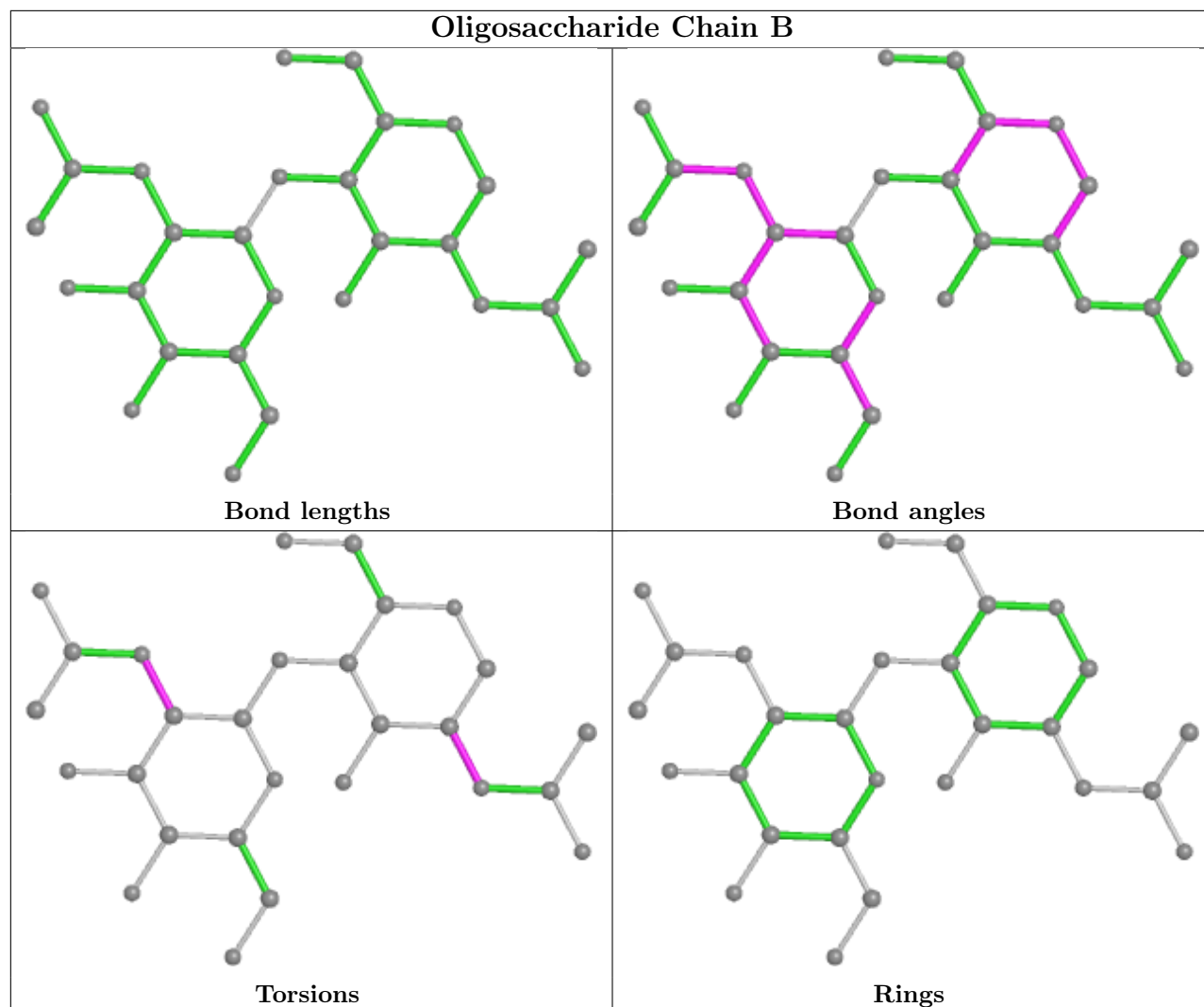
All (4) torsion outliers are listed below:

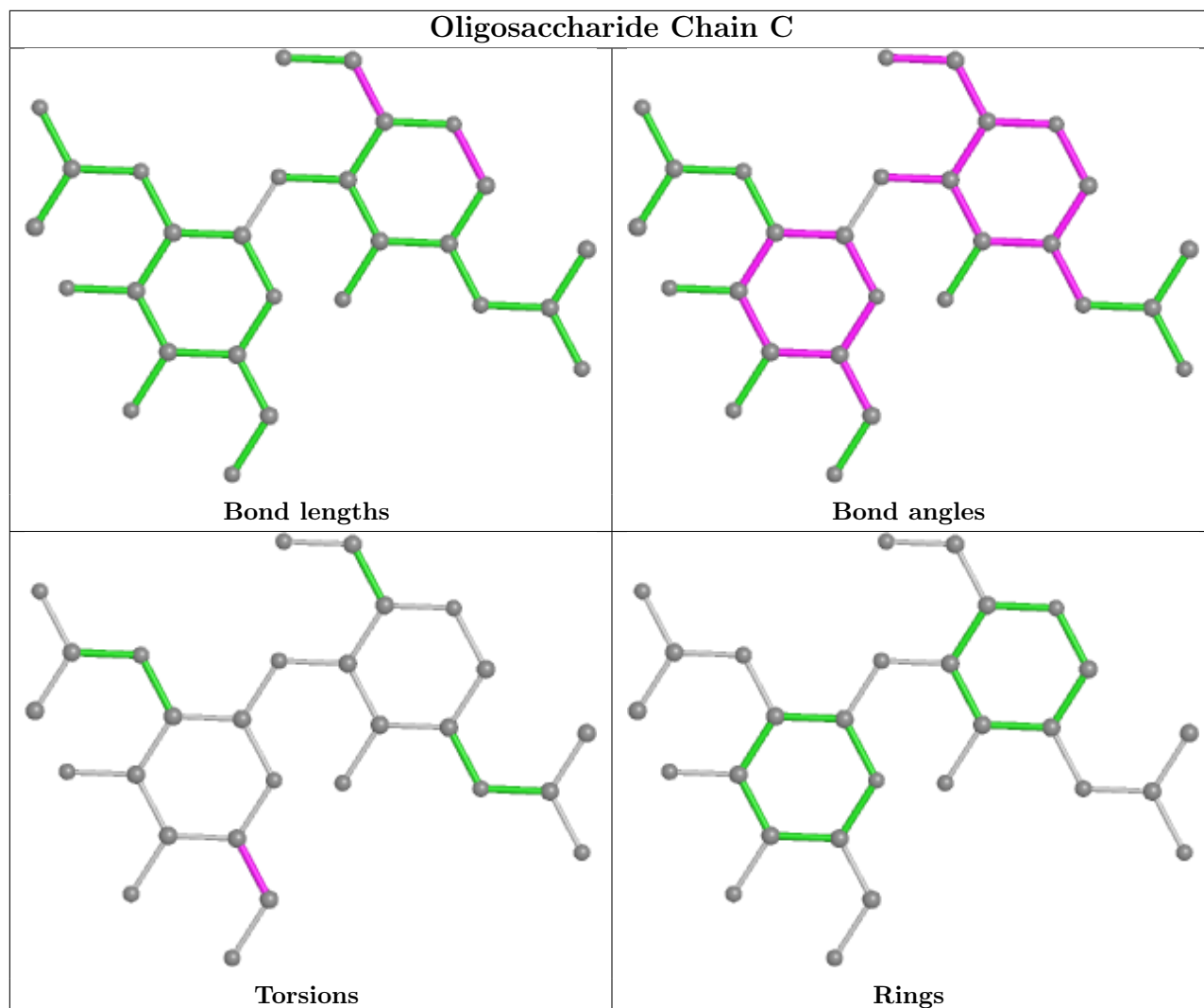
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	B	2	NAG	C3-C2-N2-C7
2	B	1	NAG	C3-C2-N2-C7

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	EPE	A	1407	-	15,15,15	2.03	1 (6%)	18,20,20	1.48	4 (22%)
3	MAN	A	1405	1	11,11,12	0.33	0	15,15,17	1.48	2 (13%)
3	MAN	A	1408	1	11,11,12	0.63	0	15,15,17	1.94	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MAN	A	1406	1	11,11,12	0.52	0	15,15,17	0.94	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	EPE	A	1407	-	-	4/9/19/19	0/1/1/1
3	MAN	A	1405	1	-	1/2/19/22	0/1/1/1
3	MAN	A	1408	1	-	1/2/19/22	0/1/1/1
3	MAN	A	1406	1	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1407	EPE	C10-S	-7.48	1.66	1.77

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1408	MAN	O5-C1-C2	-4.44	103.92	110.77
4	A	1407	EPE	O3S-S-C10	3.90	112.08	105.77
3	A	1408	MAN	C3-C4-C5	-2.94	104.99	110.24
3	A	1405	MAN	O5-C1-C2	-2.90	106.30	110.77
3	A	1408	MAN	O2-C2-C1	-2.73	103.56	109.15
4	A	1407	EPE	C5-N4-C3	2.55	114.56	108.83
3	A	1405	MAN	O6-C6-C5	-2.34	103.27	111.29
3	A	1408	MAN	O5-C5-C6	2.22	110.68	107.20
4	A	1407	EPE	C6-N1-C2	2.07	113.48	108.83
3	A	1408	MAN	O4-C4-C5	2.04	114.37	109.30
4	A	1407	EPE	O3S-S-O2S	-2.04	106.28	111.27

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1408	MAN	C4-C5-C6-O6
3	A	1405	MAN	O5-C5-C6-O6
4	A	1407	EPE	S-C10-C9-N1
4	A	1407	EPE	C9-C10-S-O1S

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Mol	Chain	Res	Type	Atoms
4	A	1407	EPE	C9-C10-S-O2S
4	A	1407	EPE	C9-C10-S-O3S

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1405	MAN	1	0
3	A	1408	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	443/474 (93%)	-0.28	0 <a href="#">100</a> <a href="#">100</a>	65, 94, 133, 163	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](#)

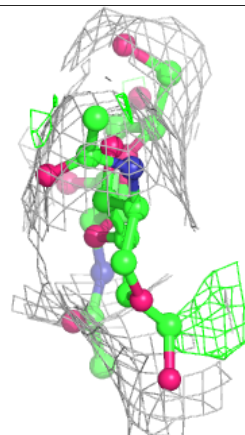
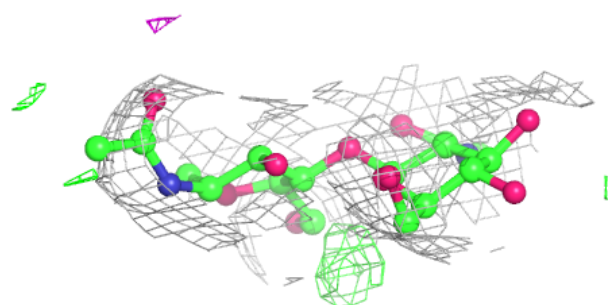
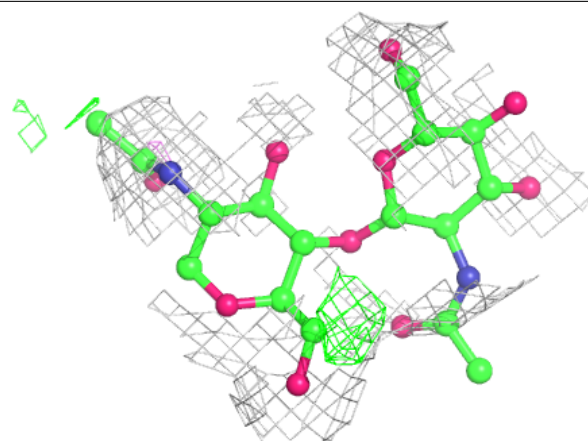
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

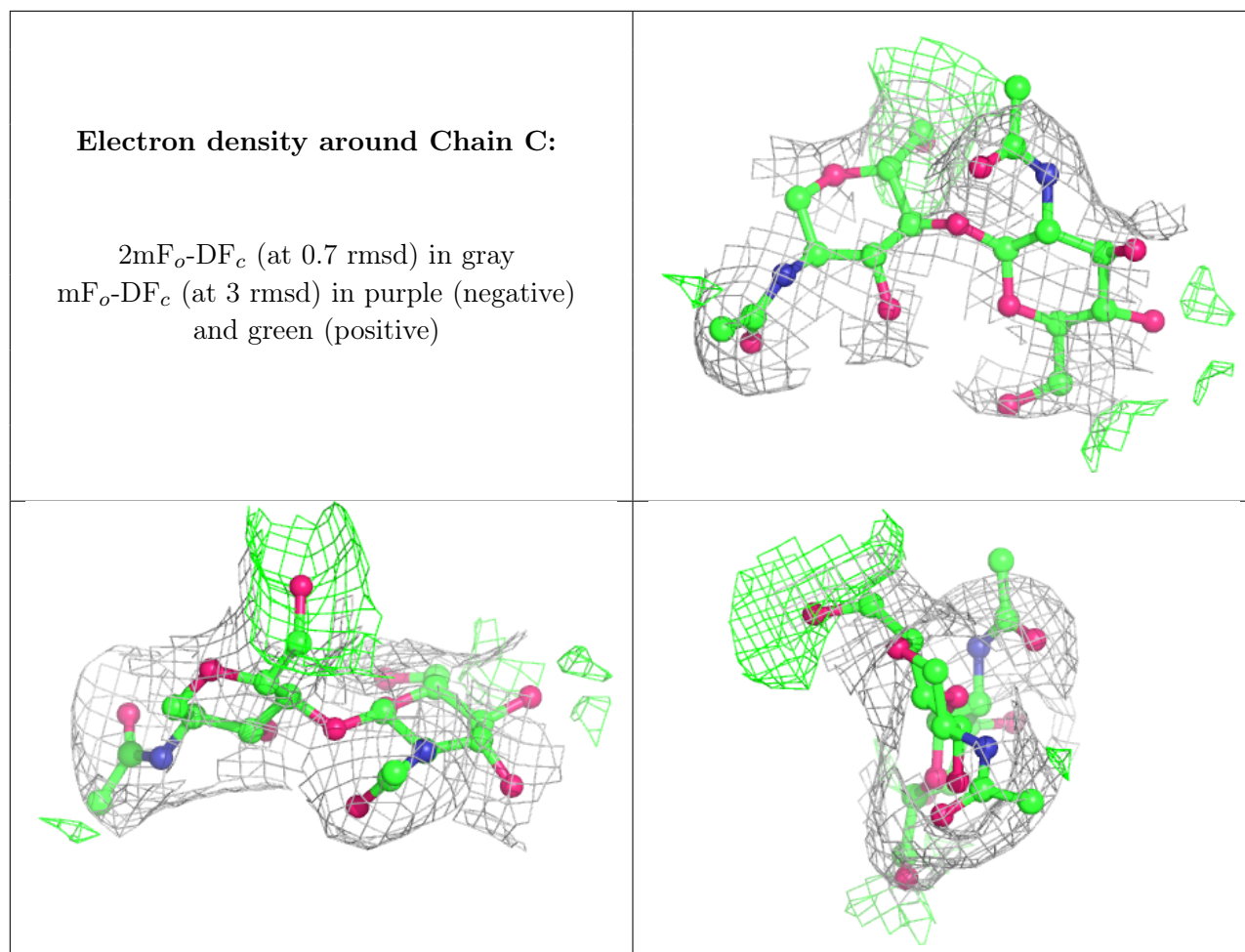
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	C	1	14/15	0.77	0.17	78,113,132,150	0
2	NAG	B	2	14/15	0.84	0.21	139,165,170,175	0
2	NAG	C	2	14/15	0.89	0.17	123,159,166,167	0
2	NAG	B	1	14/15	0.95	0.11	117,147,156,160	0

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 B:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EPE	A	1407	15/15	0.91	0.25	110,116,134,136	0
3	MAN	A	1408	11/12	0.93	0.18	90,102,127,139	0
3	MAN	A	1405	11/12	0.93	0.12	102,116,123,123	0
3	MAN	A	1406	11/12	0.94	0.15	98,102,111,112	0
5	CA	A	1411	1/1	0.97	0.04	112,112,112,112	0
5	CA	A	1410	1/1	0.99	0.10	90,90,90,90	0
5	CA	A	1409	1/1	0.99	0.07	78,78,78,78	0
5	CA	A	1412	1/1	0.99	0.14	92,92,92,92	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.