



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 06:37 PM BST

PDB ID : 2X1X  
Title : CRYSTAL STRUCTURE OF VEGF-C IN COMPLEX WITH DOMAINS 2 AND 3 OF VEGFR2 IN A TETRAGONAL CRYSTAL FORM  
Authors : Leppanen, V.-M.; Prota, A.E.; Jeltsch, M.; Anisimov, A.; Kalkkinen, N.; Strandin, T.; Lankinen, H.; Goldman, A.; Ballmer-Hofer, K.; Alitalo, K.  
Deposited on : 2010-01-08  
Resolution : 3.10 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.

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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 : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

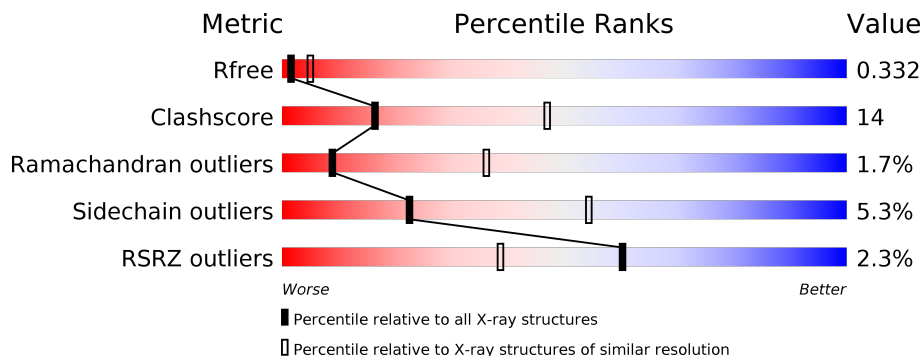
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	E	110	
2	R	213	
3	A	3	
3	B	3	
4	C	2	
4	D	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
3	NAG	A	2	-	-	-	X
3	BMA	B	3	-	-	-	X
6	NAG	R	404	X	-	-	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 2488 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 VASCULAR ENDOTHELIAL GROWTH FACTOR C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	103	779	485	135	148	11	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	137	ALA	CYS	engineered mutation	UNP P49767

- Molecule 2 is a protein called VASCULAR ENDOTHELIAL GROWTH FACTOR RECEPTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	R	201	1548	984	262	292	10	0	0	0

- Molecule 3 is an oligosaccharide called 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
			Total	C	N	O			
3	A	3	39	22	2	15	0	0	0
3	B	3	39	22	2	15	0	0	0

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

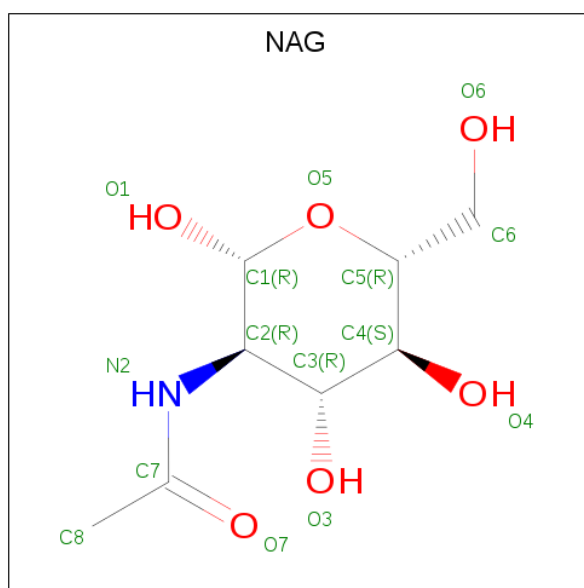


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	R	1	Total	Hg	0	0
			1	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	R	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	4	Total	O	0	0
			4	4		

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	R	8	Total	O	0	0
			8	8		

### 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.

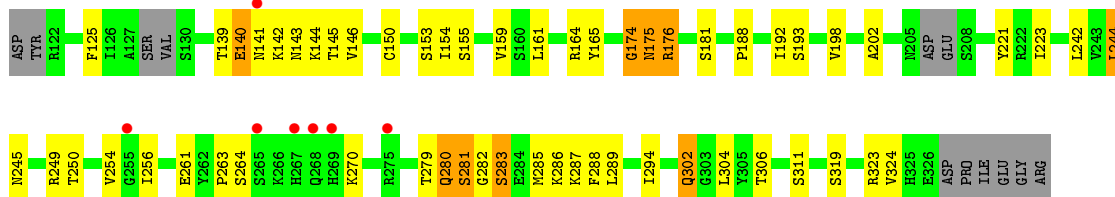
- Molecule 1: VASCULAR ENDOTHELIAL GROWTH FACTOR C

Chain E: 



- Molecule 2: VASCULAR ENDOTHELIAL GROWTH FACTOR RECEPTOR 2

Chain R: 

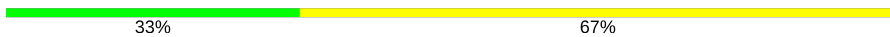


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A: 



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

Chain B: 



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

Chain C: 



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

Chain D: A horizontal progress bar for Chain D. The left half (50%) is green, and the right half (50%) is yellow. The labels '50%' are placed at the midpoint of each color segment.





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.73Å 88.73Å 105.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.00 – 3.10 67.85 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.00-3.10) 99.9 (67.85-3.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.93 (at 3.13Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.266 , 0.334 0.258 , 0.332	Depositor DCC
$R_{free}$ test set	810 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.9	Xtrriage
Anisotropy	0.360	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 60.2	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	0.87	EDS
Total number of atoms	2488	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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: BMA, NAG, HG

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	E	0.38	0/795	0.54	0/1077
2	R	0.41	0/1577	0.54	0/2135
All	All	0.40	0/2372	0.54	0/3212

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	E	779	0	751	18	0
2	R	1548	0	1523	52	0
3	A	39	0	34	0	0
3	B	39	0	34	0	0
4	C	28	0	25	1	0
4	D	28	0	25	0	0
5	R	1	0	0	0	0
6	R	14	0	13	0	0
7	E	4	0	0	0	0
7	R	8	0	0	0	0
All	All	2488	0	2405	70	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 14.

All (70) 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)
2:R:280:GLN:HA	2:R:282:GLY:N	1.59	1.16
2:R:280:GLN:CA	2:R:282:GLY:H	1.66	1.07
1:E:194:GLN:HB3	1:E:195:GLY:HA3	1.36	1.04
2:R:279:THR:O	2:R:281:SER:HB3	1.62	1.00
2:R:280:GLN:HA	2:R:282:GLY:H	0.83	0.97
1:E:194:GLN:CB	1:E:195:GLY:HA3	2.07	0.83
2:R:140:GLU:HB2	2:R:221:TYR:HE2	1.49	0.77
2:R:142:LYS:HB3	2:R:143:ASN:HA	1.68	0.76
1:E:146:VAL:HG23	1:E:147:ALA:H	1.51	0.75
2:R:264:SER:O	2:R:270:LYS:HE3	1.90	0.70
1:E:160:TYR:HB2	1:E:205:ASN:HD21	1.62	0.65
2:R:250:THR:HG21	2:R:256:ILE:HD11	1.80	0.64
2:R:280:GLN:CA	2:R:282:GLY:N	2.41	0.62
1:E:194:GLN:CB	1:E:195:GLY:CA	2.77	0.62
2:R:245:ASN:ND2	4:C:1:NAG:C1	2.66	0.59
1:E:144:PHE:HD2	1:E:146:VAL:CG1	2.16	0.58
2:R:141:ASN:HB3	2:R:144:LYS:HA	1.85	0.57
2:R:146:VAL:HG11	2:R:192:ILE:HD11	1.88	0.56
2:R:141:ASN:HB2	2:R:142:LYS:HA	1.88	0.55
2:R:141:ASN:H	2:R:141:ASN:HD22	1.53	0.55
1:E:144:PHE:HD2	1:E:146:VAL:HG12	1.72	0.55
2:R:279:THR:O	2:R:281:SER:CB	2.46	0.55
2:R:164:ARG:HD3	2:R:165:TYR:CZ	2.42	0.54
2:R:280:GLN:H	2:R:280:GLN:CD	2.10	0.54
1:E:190:VAL:HA	1:E:191:PRO:C	2.28	0.54
1:E:146:VAL:HG23	1:E:147:ALA:N	2.24	0.51
2:R:280:GLN:HB3	2:R:282:GLY:HA2	1.91	0.51
2:R:250:THR:CG2	2:R:256:ILE:HD11	2.39	0.51
2:R:280:GLN:CB	2:R:282:GLY:H	2.22	0.51
2:R:261:GLU:OE2	2:R:261:GLU:HA	2.11	0.51
2:R:141:ASN:H	2:R:141:ASN:ND2	2.09	0.50
2:R:302:GLN:HG3	2:R:324:VAL:H	1.75	0.50
2:R:280:GLN:HB3	2:R:282:GLY:N	2.25	0.50
2:R:282:GLY:O	2:R:283:SER:O	2.29	0.50
2:R:145:THR:HA	2:R:188:PRO:HA	1.93	0.49
2:R:280:GLN:CB	2:R:282:GLY:N	2.75	0.49
1:E:170:GLY:H	1:E:214:LYS:HE3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:140:GLU:CB	2:R:221:TYR:HE2	2.23	0.49
1:E:138:ILE:CG2	1:E:143:GLU:HG3	2.43	0.48
1:E:178:THR:HG23	1:E:206:HIS:HD2	1.77	0.48
1:E:138:ILE:HG23	1:E:143:GLU:HG3	1.94	0.48
2:R:142:LYS:CB	2:R:143:ASN:HA	2.41	0.48
2:R:280:GLN:HB3	2:R:282:GLY:CA	2.43	0.48
2:R:155:SER:HA	2:R:181:SER:OG	2.14	0.47
1:E:175:ASN:ND2	1:E:178:THR:OG1	2.46	0.47
2:R:242:LEU:HD11	2:R:244:LEU:HD13	1.97	0.47
2:R:223:ILE:HA	2:R:250:THR:HG22	1.97	0.46
2:R:174:GLY:HA2	2:R:175:ASN:HA	1.50	0.46
2:R:154:ILE:HG22	2:R:155:SER:N	2.31	0.46
1:E:205:ASN:C	1:E:205:ASN:HD22	2.20	0.45
2:R:242:LEU:HD23	2:R:294:ILE:HD12	1.98	0.45
2:R:306:THR:HG23	2:R:319:SER:HB3	1.99	0.44
2:R:249:ARG:HD3	2:R:287:LYS:HE2	1.99	0.44
2:R:286:LYS:HD3	2:R:288:PHE:HZ	1.82	0.44
2:R:250:THR:OG1	2:R:288:PHE:HE1	1.99	0.44
2:R:263:PRO:HD3	2:R:304:LEU:O	2.17	0.44
1:E:194:GLN:HB3	1:E:195:GLY:CA	2.25	0.44
2:R:302:GLN:HG3	2:R:323:ARG:HA	1.99	0.43
2:R:159:VAL:HG22	2:R:202:ALA:HB2	2.00	0.43
2:R:245:ASN:ND2	2:R:289:LEU:HD11	2.34	0.42
2:R:125:PHE:CE1	2:R:150:CYS:HB3	2.54	0.42
2:R:175:ASN:O	2:R:176:ARG:HB2	2.20	0.42
2:R:153:SER:HB2	2:R:154:ILE:HD12	2.01	0.42
2:R:161:LEU:HD11	2:R:198:VAL:HB	2.02	0.42
1:E:160:TYR:HB2	1:E:205:ASN:ND2	2.32	0.42
1:E:144:PHE:HB3	1:E:146:VAL:HG13	2.01	0.42
2:R:254:VAL:HG13	2:R:311:SER:HB2	2.01	0.41
2:R:279:THR:OG1	2:R:285:MET:O	2.31	0.41
2:R:125:PHE:HE1	2:R:150:CYS:HB3	1.85	0.40
2:R:143:ASN:C	2:R:145:THR:H	2.23	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	E	101/110 (92%)	96 (95%)	4 (4%)	1 (1%)	15	49
2	R	195/213 (92%)	180 (92%)	11 (6%)	4 (2%)	7	30
All	All	296/323 (92%)	276 (93%)	15 (5%)	5 (2%)	9	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	146	VAL
2	R	283	SER
2	R	176	ARG
2	R	174	GLY
2	R	281	SER

### 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	E	90/100 (90%)	83 (92%)	7 (8%)	12	40
2	R	173/192 (90%)	166 (96%)	7 (4%)	31	65
All	All	263/292 (90%)	249 (95%)	14 (5%)	22	54

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	120	LYS

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Mol	Chain	Res	Type
1	E	123	ASP
1	E	126	TRP
1	E	144	PHE
1	E	192	LEU
1	E	194	GLN
1	E	205	ASN
2	R	139	THR
2	R	140	GLU
2	R	175	ASN
2	R	193	SER
2	R	244	LEU
2	R	280	GLN
2	R	302	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	115	ASN
1	E	175	ASN
1	E	205	ASN
2	R	141	ASN
2	R	175	ASN
2	R	245	ASN
2	R	325	HIS

### 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](#)

10 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
3	NAG	A	1	3	14,14,15	0.59	0	17,19,21	1.67	2 (11%)
3	NAG	A	2	3	14,14,15	0.51	0	17,19,21	1.06	1 (5%)
3	BMA	A	3	3	11,11,12	0.69	0	15,15,17	0.93	1 (6%)
3	NAG	B	1	3	14,14,15	0.40	0	17,19,21	1.12	2 (11%)
3	NAG	B	2	3	14,14,15	0.60	0	17,19,21	1.02	1 (5%)
3	BMA	B	3	3	11,11,12	0.74	0	15,15,17	0.79	0
4	NAG	C	1	4	14,14,15	0.57	0	17,19,21	1.13	0
4	NAG	C	2	4	14,14,15	0.48	0	17,19,21	0.90	0
4	NAG	D	1	4	14,14,15	0.71	0	17,19,21	1.47	3 (17%)
4	NAG	D	2	4	14,14,15	0.54	0	17,19,21	0.71	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
3	NAG	A	1	3	-	1/6/23/26	0/1/1/1
3	NAG	A	2	3	-	4/6/23/26	0/1/1/1
3	BMA	A	3	3	-	0/2/19/22	0/1/1/1
3	NAG	B	1	3	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
3	BMA	B	3	3	-	2/2/19/22	0/1/1/1
4	NAG	C	1	4	-	3/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	NAG	D	1	4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	NAG	C3-C4-C5	4.18	117.69	110.24
3	A	1	NAG	O5-C1-C2	-3.98	105.01	111.29
4	D	1	NAG	C4-C3-C2	3.19	115.69	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	C3-C4-C5	2.76	115.16	110.24
4	D	1	NAG	C1-O5-C5	-2.74	108.48	112.19
3	B	2	NAG	C4-C3-C2	2.60	114.83	111.02
3	B	1	NAG	C4-C3-C2	-2.36	107.56	111.02
3	B	1	NAG	C1-O5-C5	2.24	115.22	112.19
3	A	3	BMA	C3-C4-C5	2.15	114.07	110.24
3	A	2	NAG	C4-C3-C2	-2.01	108.07	111.02

There are no chirality outliers.

All (13) torsion outliers are listed below:

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

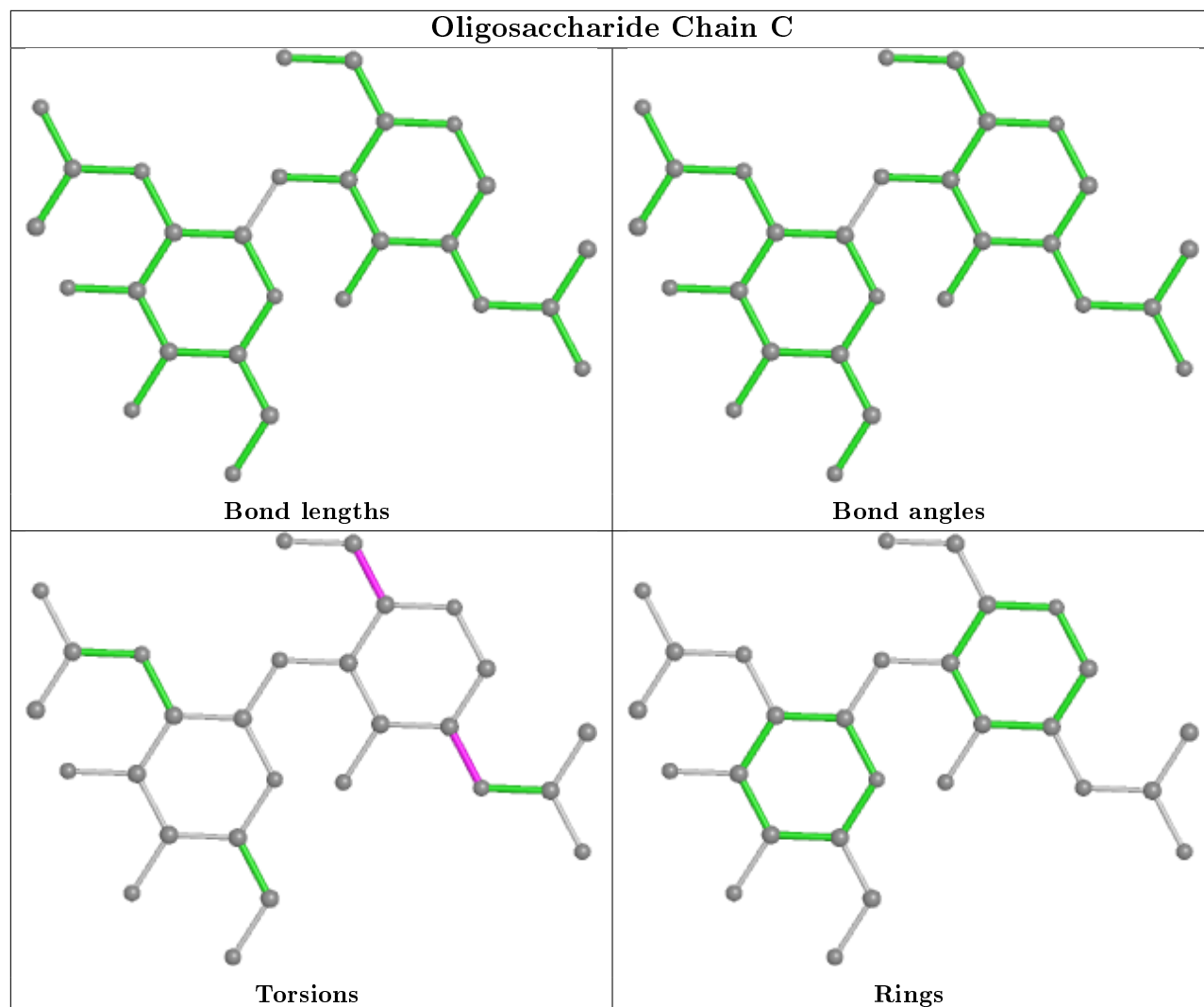
There are no ring outliers.

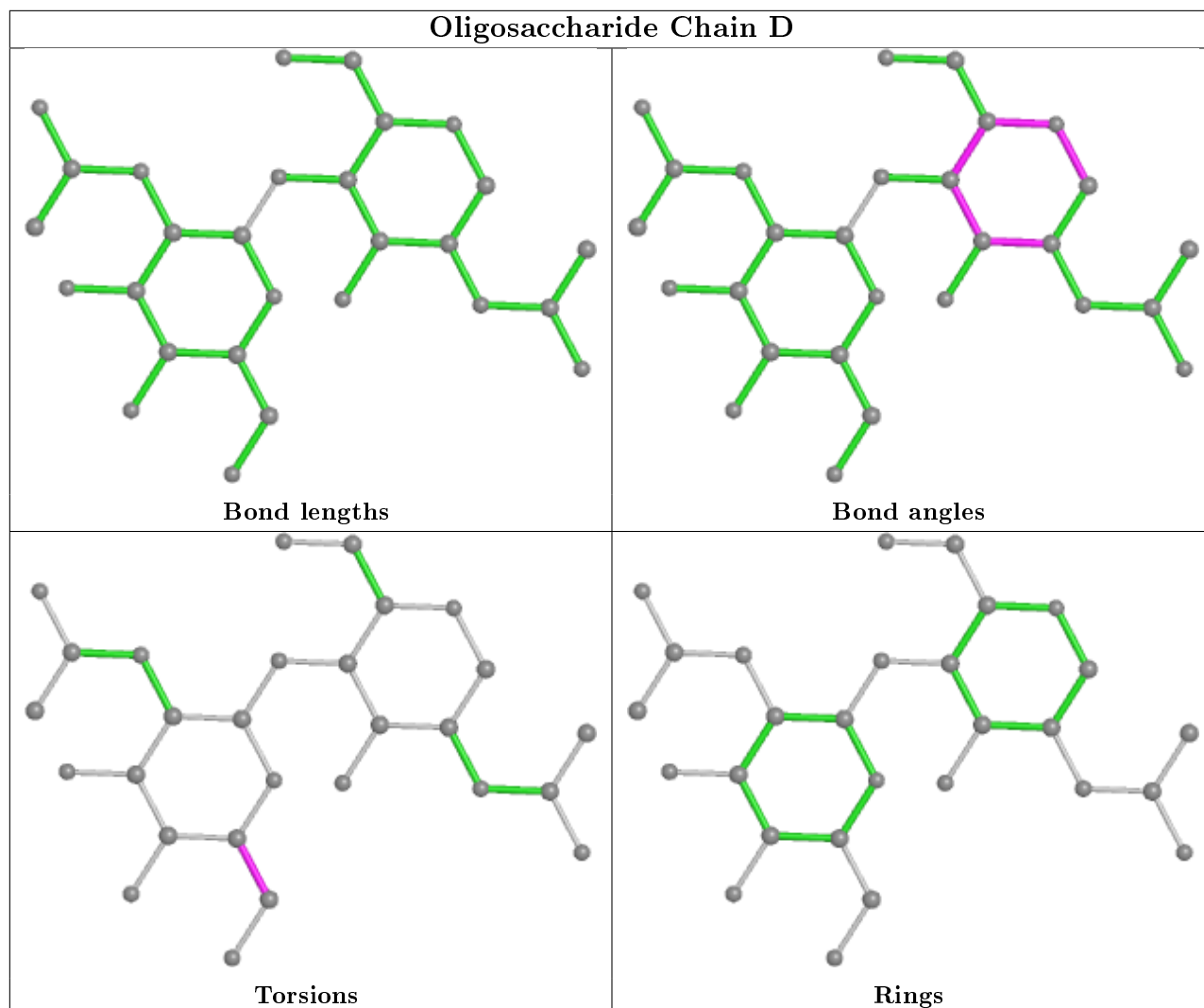
1 monomer is involved in 1 short contact:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
6	NAG	R	404	2	14,14,15	0.59	0	17,19,21	1.61	3 (17%)

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
6	NAG	R	404	2	1/1/5/7	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	404	NAG	O5-C1-C2	-4.73	103.82	111.29
6	R	404	NAG	C1-O5-C5	2.58	115.69	112.19
6	R	404	NAG	C1-C2-N2	2.38	114.56	110.49

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	R	404	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	404	NAG	O5-C5-C6-O6
6	R	404	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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	E	103/110 (93%)	0.07	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	33, 48, 71, 91	0
2	R	201/213 (94%)	0.09	7 (3%) <span style="border: 1px solid red; padding: 2px;">44</span> <span style="border: 1px solid red; padding: 2px;">23</span>	26, 54, 81, 99	0
All	All	304/323 (94%)	0.08	7 (2%) <span style="border: 1px solid blue; padding: 2px;">60</span> <span style="border: 1px solid red; padding: 2px;">39</span>	26, 52, 79, 99	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	141	ASN	3.9
2	R	268	GLN	3.6
2	R	267	HIS	3.5
2	R	275	ARG	2.8
2	R	265	SER	2.4
2	R	255	GLY	2.2
2	R	269	HIS	2.2

### 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.

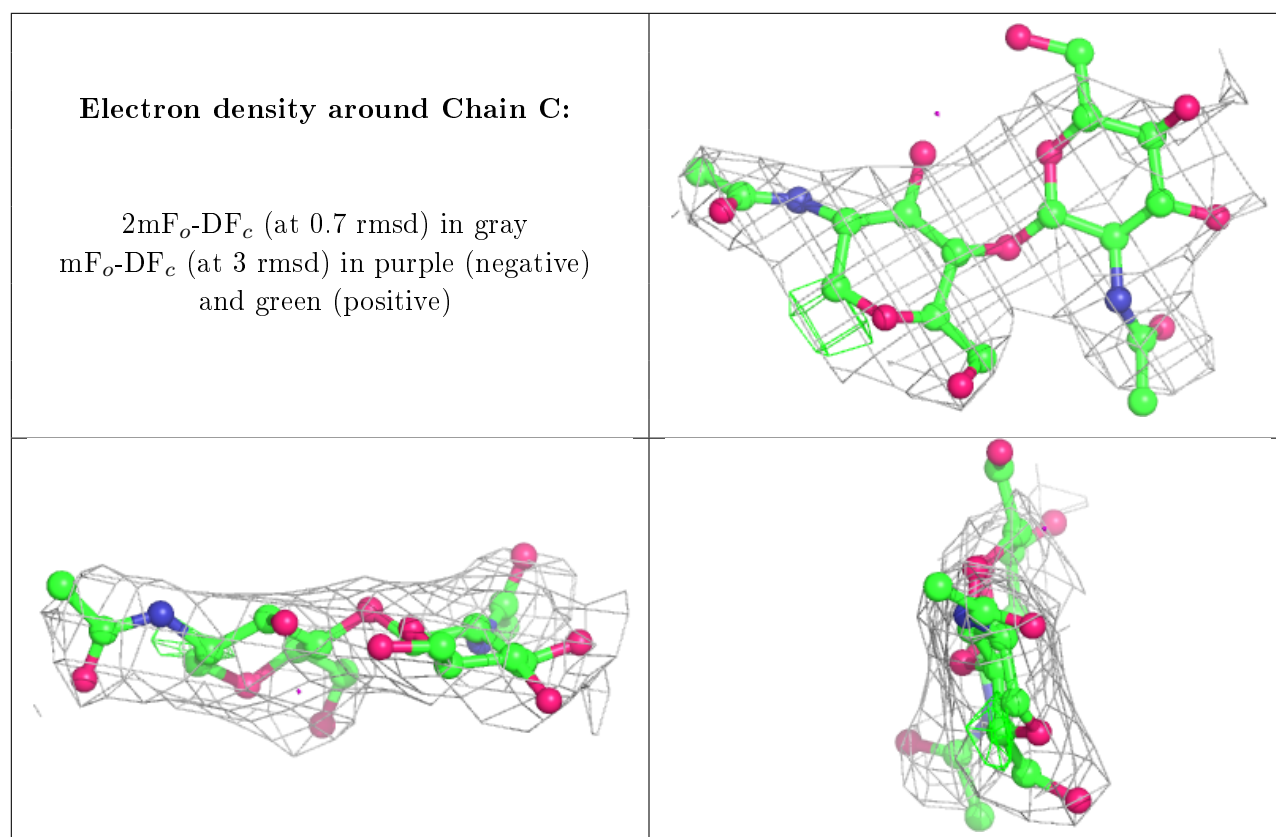
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	BMA	B	3	11/12	<span style="background-color: yellow;">0.53</span>	<span style="background-color: yellow;">0.44</span>	86,89,92,92	0
3	BMA	A	3	11/12	0.54	0.34	112,114,115,116	0

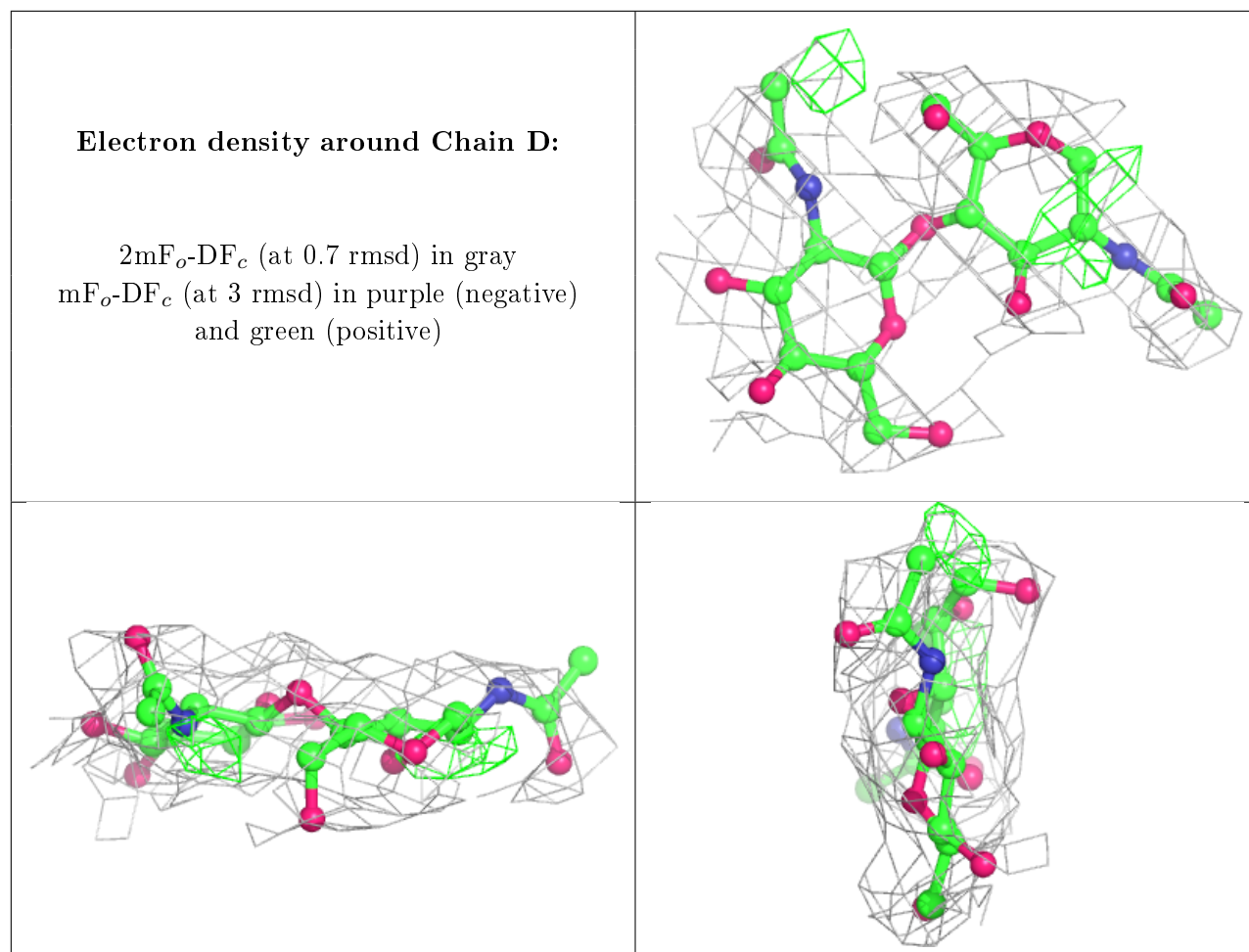
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	2	14/15	0.57	0.42	98,102,106,110	0
4	NAG	D	2	14/15	0.79	0.18	107,108,109,109	0
3	NAG	B	1	14/15	0.80	0.33	72,76,77,77	0
4	NAG	C	2	14/15	0.83	0.34	84,86,89,89	0
3	NAG	A	1	14/15	0.83	0.30	72,83,87,94	0
4	NAG	D	1	14/15	0.84	0.27	99,101,104,105	0
3	NAG	B	2	14/15	0.85	0.24	74,76,78,82	0
4	NAG	C	1	14/15	0.88	0.27	73,76,78,80	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, 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
6	NAG	R	404	14/15	0.68	0.28	90,93,96,97	0
5	HG	R	401	1/1	0.98	0.07	140,140,140,140	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.