



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 04:18 AM EDT

PDB ID : 5MYA
Title : Homodimerization of Tie2 Fibronectin-like domains 1-3 in space group C2
Authors : Leppanen, V.-M.; Saharinen, P.; Alitalo, K.
Deposited on : 2017-01-26
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

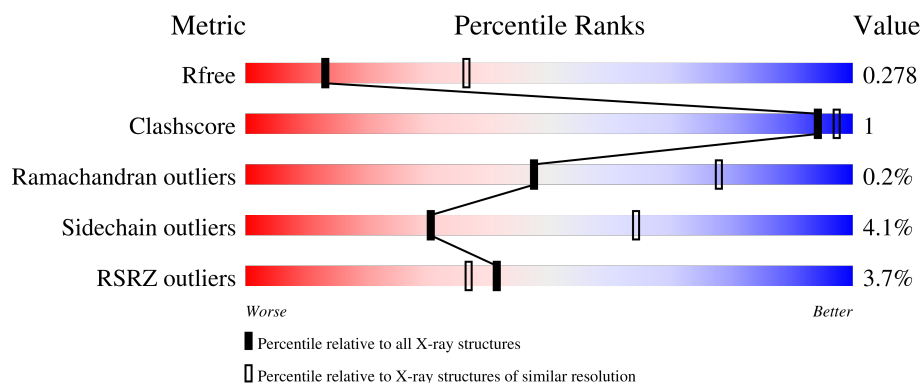
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	333	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>5%</div> <div>12%</div> </div> </div>
1	B	333	<div> <div>4%</div> <div> <div></div> <div>53%</div> <div>•</div> <div>43%</div> </div> </div>
2	C	2	<div> <div></div> <div>100%</div> </div>
3	D	4	<div> <div>25%</div> <div>75%</div> </div>
4	E	3	<div> <div>67%</div> <div>33%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3972 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 Angiopoietin-1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2282	1451	393	437	1			
1	B	191	Total	C	N	O		0	0	0
			1454	917	254	283				

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	MET	-	initiating methionine	UNP Q02763
A	421	LYS	-	expression tag	UNP Q02763
A	422	PHE	-	expression tag	UNP Q02763
A	423	LEU	-	expression tag	UNP Q02763
A	424	VAL	-	expression tag	UNP Q02763
A	425	ASN	-	expression tag	UNP Q02763
A	426	VAL	-	expression tag	UNP Q02763
A	427	ALA	-	expression tag	UNP Q02763
A	428	LEU	-	expression tag	UNP Q02763
A	429	VAL	-	expression tag	UNP Q02763
A	430	PHE	-	expression tag	UNP Q02763
A	431	MET	-	expression tag	UNP Q02763
A	432	VAL	-	expression tag	UNP Q02763
A	433	VAL	-	expression tag	UNP Q02763
A	434	TYR	-	expression tag	UNP Q02763
A	435	ILE	-	expression tag	UNP Q02763
A	436	SER	-	expression tag	UNP Q02763
A	437	TYR	-	expression tag	UNP Q02763
A	438	ILE	-	expression tag	UNP Q02763
A	439	TYR	-	expression tag	UNP Q02763
A	440	ALA	-	expression tag	UNP Q02763
A	441	ASP	-	expression tag	UNP Q02763
A	442	PRO	-	expression tag	UNP Q02763
A	743	ILE	-	expression tag	UNP Q02763
A	744	GLU	-	expression tag	UNP Q02763

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	745	GLY	-	expression tag	UNP Q02763
A	746	ARG	-	expression tag	UNP Q02763
A	747	HIS	-	expression tag	UNP Q02763
A	748	HIS	-	expression tag	UNP Q02763
A	749	HIS	-	expression tag	UNP Q02763
A	750	HIS	-	expression tag	UNP Q02763
A	751	HIS	-	expression tag	UNP Q02763
A	752	HIS	-	expression tag	UNP Q02763
B	420	MET	-	initiating methionine	UNP Q02763
B	421	LYS	-	expression tag	UNP Q02763
B	422	PHE	-	expression tag	UNP Q02763
B	423	LEU	-	expression tag	UNP Q02763
B	424	VAL	-	expression tag	UNP Q02763
B	425	ASN	-	expression tag	UNP Q02763
B	426	VAL	-	expression tag	UNP Q02763
B	427	ALA	-	expression tag	UNP Q02763
B	428	LEU	-	expression tag	UNP Q02763
B	429	VAL	-	expression tag	UNP Q02763
B	430	PHE	-	expression tag	UNP Q02763
B	431	MET	-	expression tag	UNP Q02763
B	432	VAL	-	expression tag	UNP Q02763
B	433	VAL	-	expression tag	UNP Q02763
B	434	TYR	-	expression tag	UNP Q02763
B	435	ILE	-	expression tag	UNP Q02763
B	436	SER	-	expression tag	UNP Q02763
B	437	TYR	-	expression tag	UNP Q02763
B	438	ILE	-	expression tag	UNP Q02763
B	439	TYR	-	expression tag	UNP Q02763
B	440	ALA	-	expression tag	UNP Q02763
B	441	ASP	-	expression tag	UNP Q02763
B	442	PRO	-	expression tag	UNP Q02763
B	743	ILE	-	expression tag	UNP Q02763
B	744	GLU	-	expression tag	UNP Q02763
B	745	GLY	-	expression tag	UNP Q02763
B	746	ARG	-	expression tag	UNP Q02763
B	747	HIS	-	expression tag	UNP Q02763
B	748	HIS	-	expression tag	UNP Q02763
B	749	HIS	-	expression tag	UNP Q02763
B	750	HIS	-	expression tag	UNP Q02763
B	751	HIS	-	expression tag	UNP Q02763
B	752	HIS	-	expression tag	UNP Q02763

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

cetamido-2-deoxy-beta-D-glucopyranose.



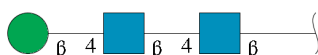
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



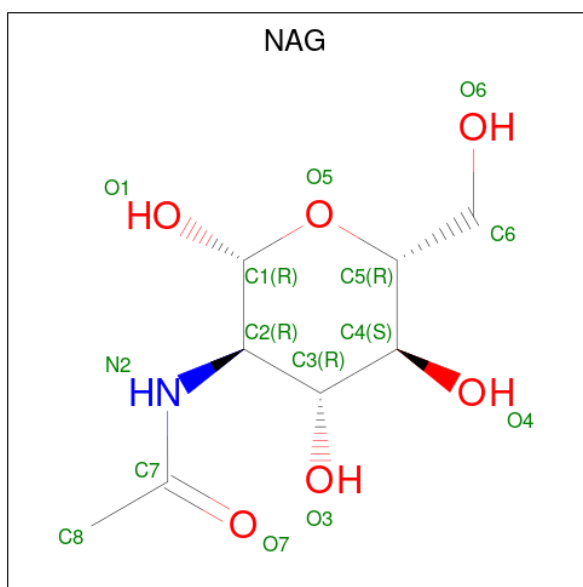
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 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
4	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

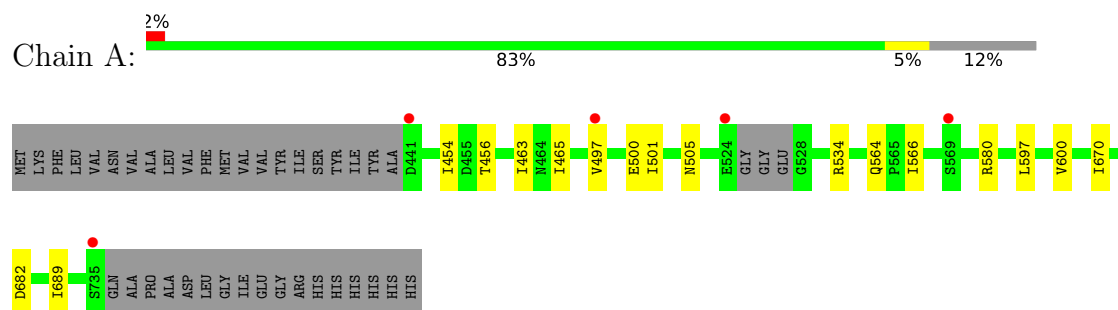
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	48	Total	O	0	0
			48	48		
6	B	15	Total	O	0	0
			15	15		

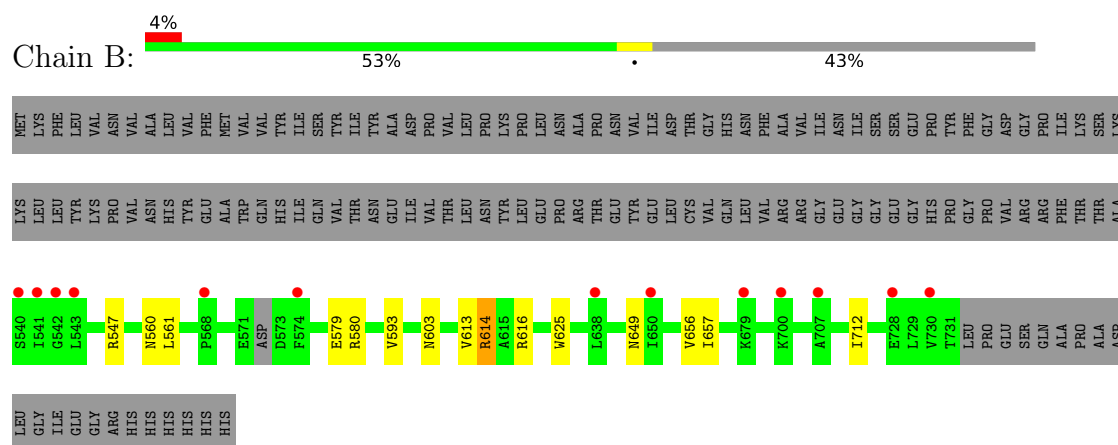
3 Residue-property plots [i](#)

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: Angiopoietin-1 receptor



- Molecule 1: Angiopoietin-1 receptor



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



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





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

Chain E:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	134.16Å 104.69Å 79.52Å 90.00° 121.41° 90.00°	Depositor
Resolution (Å)	29.42 – 2.90 29.42 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.42-2.90) 100.0 (29.42-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.234 , 0.277 0.235 , 0.278	Depositor DCC
R_{free} test set	1075 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	110.3	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 82.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3972	wwPDB-VP
Average B, all atoms (Å ²)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, NAG

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	0/2339	0.56	0/3204
1	B	0.34	0/1485	0.54	0/2038
All	All	0.34	0/3824	0.55	0/5242

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	2282	0	2231	4	0
1	B	1454	0	1400	6	0
2	C	28	0	25	0	0
3	D	50	0	43	0	0
4	E	39	0	34	0	0
5	A	28	0	26	0	0
5	B	28	0	26	0	0
6	A	48	0	0	0	0
6	B	15	0	0	0	0
All	All	3972	0	3785	10	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 1.

All (10) 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:657:ILE:HD11	1:B:712:ILE:HD11	1.87	0.56
1:B:561:LEU:HD13	1:B:613:VAL:HG21	1.91	0.52
1:B:614:ARG:HD3	1:B:625:TRP:CE3	2.47	0.49
1:A:465:ILE:HD13	1:A:497:VAL:HG21	1.97	0.46
1:A:465:ILE:CD1	1:A:497:VAL:HG21	2.47	0.44
1:B:649:ASN:HB2	1:B:656:VAL:HG12	1.99	0.44
1:B:616:ARG:HG3	1:B:625:TRP:CE3	2.54	0.42
1:A:454:ILE:HD11	1:A:501:ILE:HD12	2.00	0.42
1:B:657:ILE:CD1	1:B:712:ILE:HD11	2.51	0.40
1:A:670:ILE:HD11	1:A:689:ILE:HD12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	288/333 (86%)	278 (96%)	9 (3%)	1 (0%)	41	71
1	B	187/333 (56%)	179 (96%)	8 (4%)	0	100	100
All	All	475/666 (71%)	457 (96%)	17 (4%)	1 (0%)	47	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	500	GLU

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	256/299 (86%)	246 (96%)	10 (4%)	32	66
1	B	160/299 (54%)	153 (96%)	7 (4%)	28	61
All	All	416/598 (70%)	399 (96%)	17 (4%)	30	64

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	456	THR
1	A	463	ILE
1	A	505	ASN
1	A	534	ARG
1	A	564	GLN
1	A	566	ILE
1	A	580	ARG
1	A	597	LEU
1	A	600	VAL
1	A	682	ASP
1	B	547	ARG
1	B	560	ASN
1	B	579	GLU
1	B	580	ARG
1	B	593	VAL
1	B	603	ASN
1	B	614	ARG

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	493	GLN
1	A	698	GLN
1	B	603	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

9 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	0.65	0	17,19,21	1.36	2 (11%)
2	NAG	C	2	2	14,14,15	0.43	0	17,19,21	1.43	4 (23%)
3	NAG	D	1	3,1	14,14,15	0.41	0	17,19,21	1.47	4 (23%)
3	NAG	D	2	3	14,14,15	0.41	0	17,19,21	0.71	0
3	BMA	D	3	3	11,11,12	0.94	1 (9%)	15,15,17	1.96	4 (26%)
3	MAN	D	4	3	11,11,12	0.28	0	15,15,17	0.77	1 (6%)
4	NAG	E	1	4,1	14,14,15	0.58	0	17,19,21	1.26	1 (5%)
4	NAG	E	2	4	14,14,15	0.45	0	17,19,21	0.66	0
4	BMA	E	3	4	11,11,12	0.30	0	15,15,17	0.75	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	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)
3	D	3	BMA	C2-C3	2.28	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	BMA	C1-C2-C3	5.08	115.91	109.67
2	C	1	NAG	C4-C3-C2	4.11	117.04	111.02
3	D	1	NAG	C1-O5-C5	3.80	117.34	112.19
4	E	1	NAG	O5-C5-C6	3.63	112.90	107.20
2	C	2	NAG	C1-O5-C5	3.08	116.36	112.19
3	D	3	BMA	O5-C1-C2	2.87	115.20	110.77
2	C	2	NAG	C4-C3-C2	2.67	114.93	111.02
2	C	2	NAG	C3-C4-C5	2.48	114.67	110.24
2	C	1	NAG	C1-O5-C5	2.46	115.52	112.19
3	D	4	MAN	C1-O5-C5	2.45	115.51	112.19
3	D	1	NAG	C2-N2-C7	2.39	126.31	122.90
3	D	1	NAG	C1-C2-N2	2.32	114.45	110.49
3	D	3	BMA	O5-C5-C4	-2.25	105.34	110.83
3	D	3	BMA	C2-C3-C4	2.23	114.75	110.89
2	C	2	NAG	O5-C1-C2	-2.14	107.91	111.29
3	D	1	NAG	C4-C3-C2	-2.05	108.01	111.02

There are no chirality outliers.

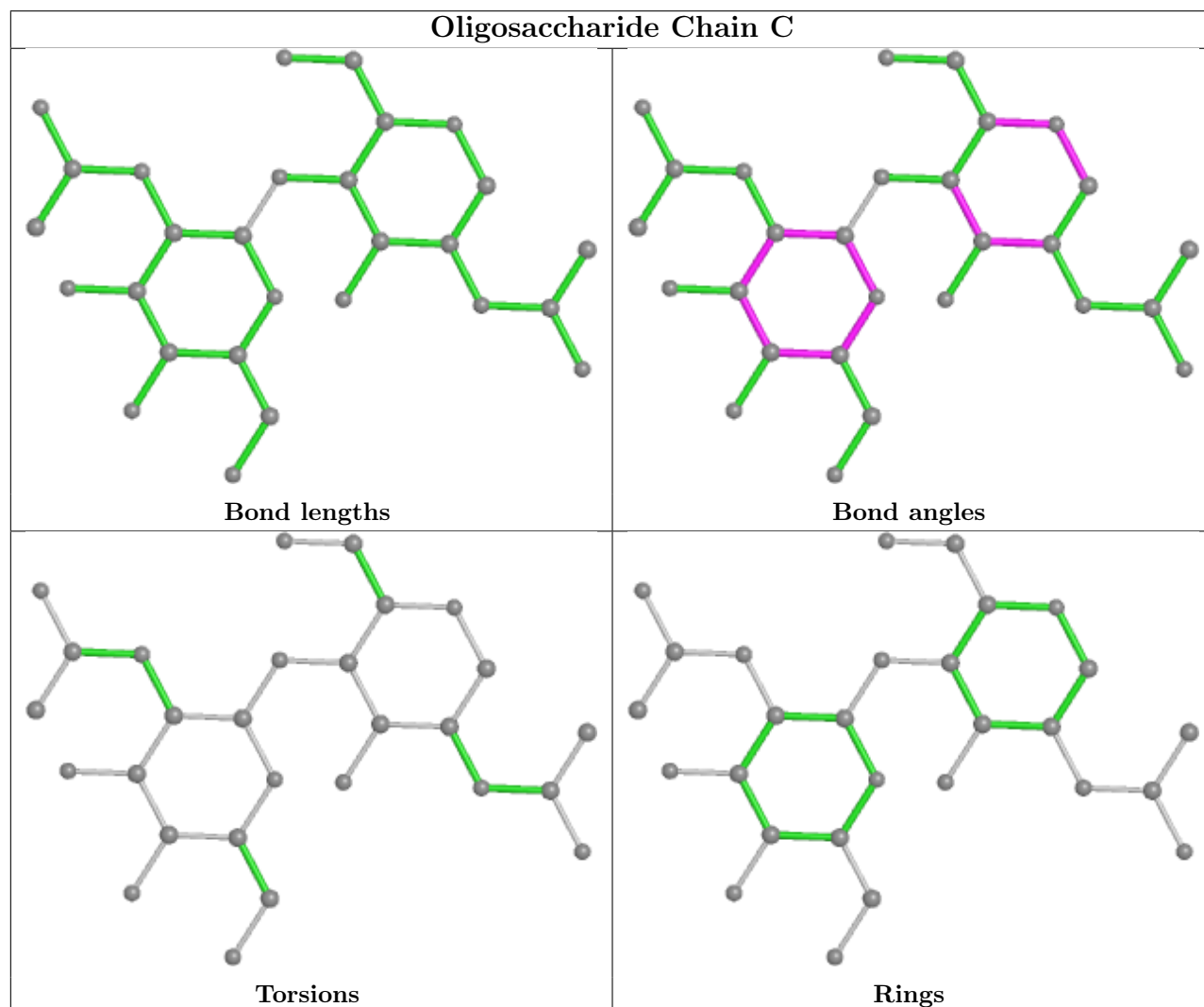
All (5) torsion outliers are listed below:

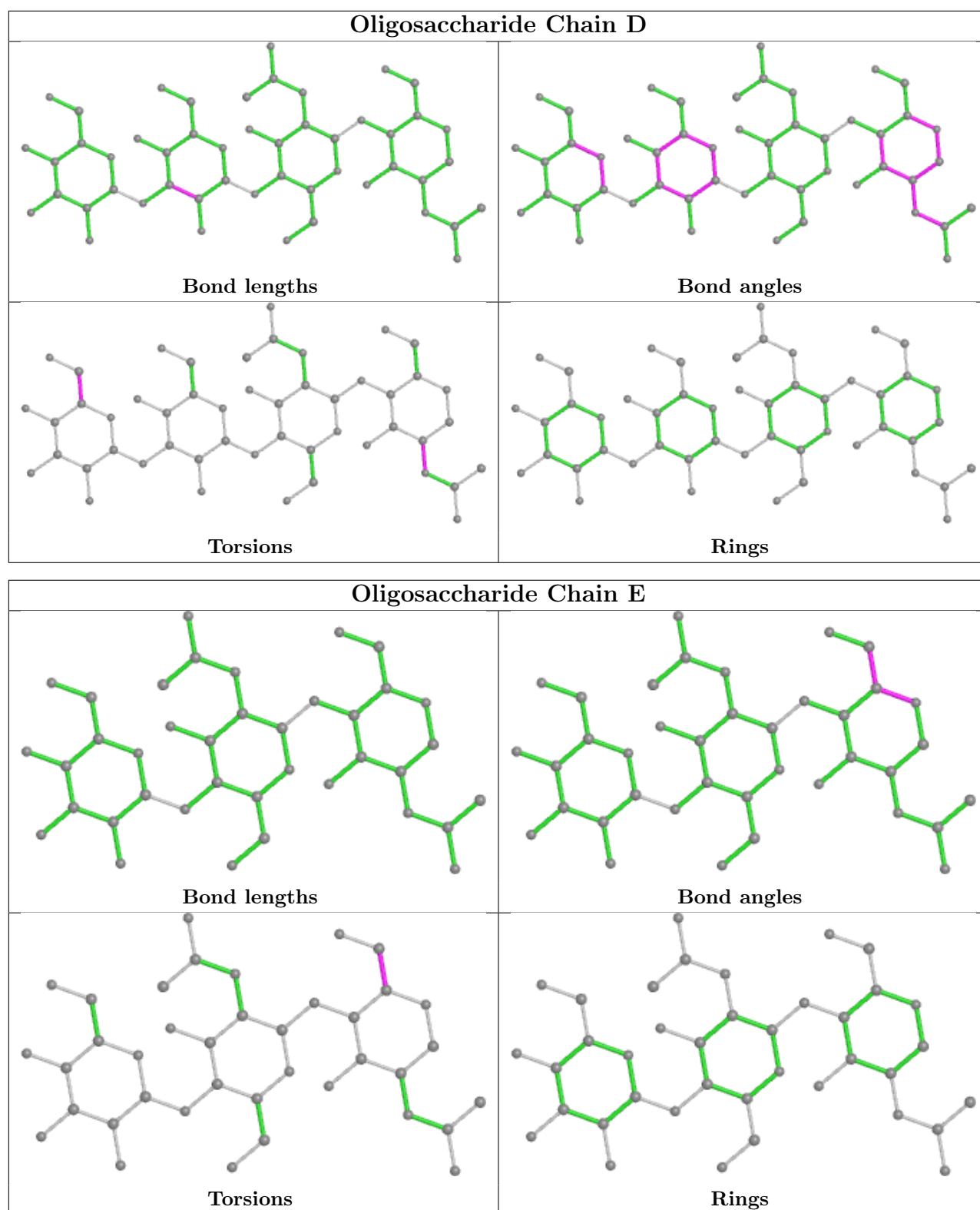
Mol	Chain	Res	Type	Atoms
3	D	4	MAN	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
3	D	1	NAG	C3-C2-N2-C7

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](#)

4 ligands 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
5	NAG	A	808	1	14,14,15	0.54	0	17,19,21	1.64	2 (11%)
5	NAG	B	805	1	14,14,15	0.34	0	17,19,21	0.81	0
5	NAG	A	807	1	14,14,15	0.31	0	17,19,21	1.18	2 (11%)
5	NAG	B	804	1	14,14,15	0.59	0	17,19,21	2.25	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
5	NAG	A	808	1	-	0/6/23/26	0/1/1/1
5	NAG	B	805	1	-	0/6/23/26	0/1/1/1
5	NAG	A	807	1	-	3/6/23/26	0/1/1/1
5	NAG	B	804	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	804	NAG	C1-O5-C5	6.53	121.04	112.19
5	A	808	NAG	C1-O5-C5	5.21	119.26	112.19
5	B	804	NAG	O5-C1-C2	4.35	118.16	111.29
5	A	808	NAG	O5-C5-C6	3.02	111.94	107.20
5	A	807	NAG	C2-N2-C7	2.99	127.16	122.90
5	B	804	NAG	C2-N2-C7	2.76	126.83	122.90
5	B	804	NAG	C8-C7-N2	2.71	120.69	116.10
5	A	807	NAG	C8-C7-N2	2.59	120.48	116.10

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	807	NAG	C8-C7-N2-C2
5	A	807	NAG	O7-C7-N2-C2
5	B	804	NAG	C8-C7-N2-C2
5	B	804	NAG	O7-C7-N2-C2
5	B	804	NAG	O5-C5-C6-O6
5	A	807	NAG	O5-C5-C6-O6
5	B	804	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, 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	292/333 (87%)	-0.20	5 (1%) 70 69	76, 121, 189, 250	0
1	B	191/333 (57%)	0.07	13 (6%) 17 13	96, 150, 221, 251	0
All	All	483/666 (72%)	-0.09	18 (3%) 41 37	76, 130, 210, 251	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	568	PRO	3.9
1	B	574	PHE	3.7
1	B	730	VAL	3.7
1	A	569	SER	3.7
1	A	441	ASP	3.6
1	B	650	ILE	3.5
1	B	543	LEU	3.3
1	B	540	SER	3.3
1	B	679	LYS	3.1
1	B	638	LEU	2.9
1	A	524	GLU	2.8
1	B	700	LYS	2.7
1	A	735	SER	2.7
1	B	728	GLU	2.7
1	B	542	GLY	2.3
1	A	497	VAL	2.2
1	B	707	ALA	2.2
1	B	541	ILE	2.0

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

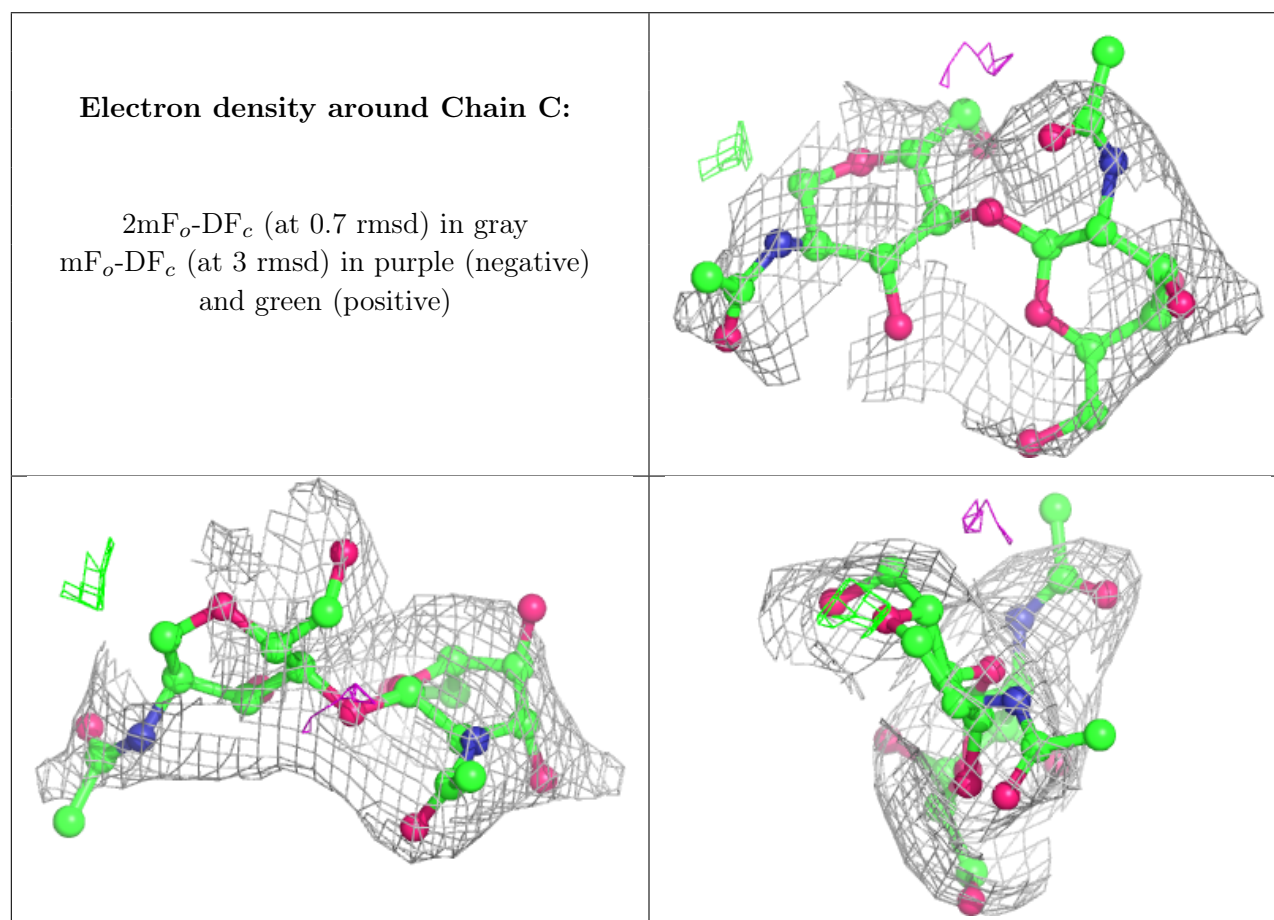
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.

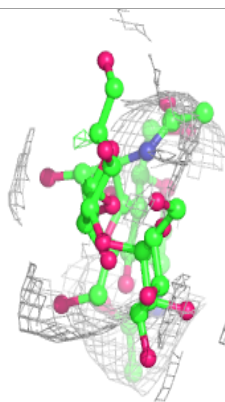
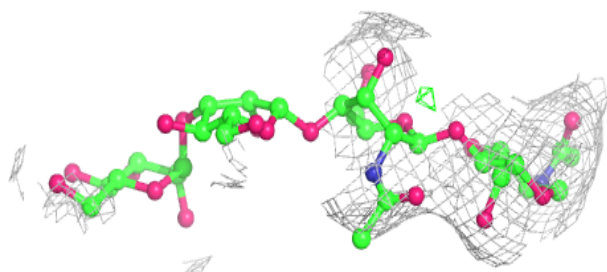
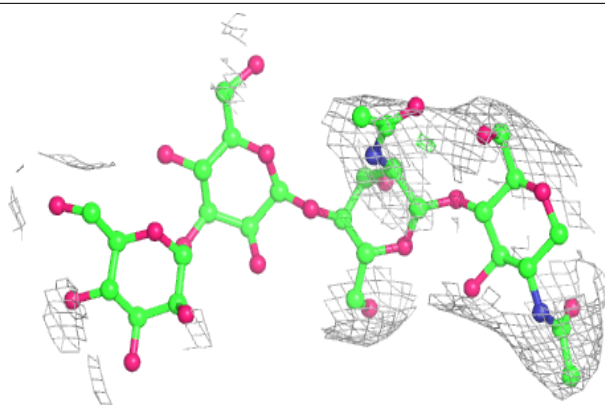
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	E	1	14/15	0.81	0.29	142,192,200,208	0
4	BMA	E	3	11/12	0.81	0.44	243,251,257,259	0
3	BMA	D	3	11/12	0.82	0.21	164,191,197,202	0
2	NAG	C	1	14/15	0.84	0.28	151,188,193,193	0
4	NAG	E	2	14/15	0.86	0.24	172,216,233,251	0
3	MAN	D	4	11/12	0.87	0.25	187,195,199,205	0
3	NAG	D	2	14/15	0.88	0.19	145,162,187,193	0
2	NAG	C	2	14/15	0.90	0.21	163,175,184,187	0
3	NAG	D	1	14/15	0.95	0.10	108,124,144,146	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

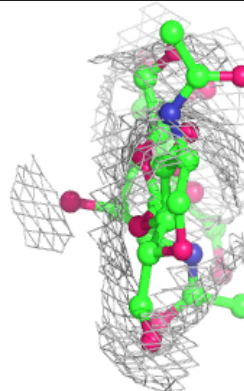
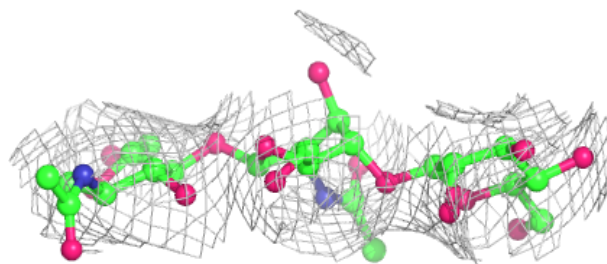
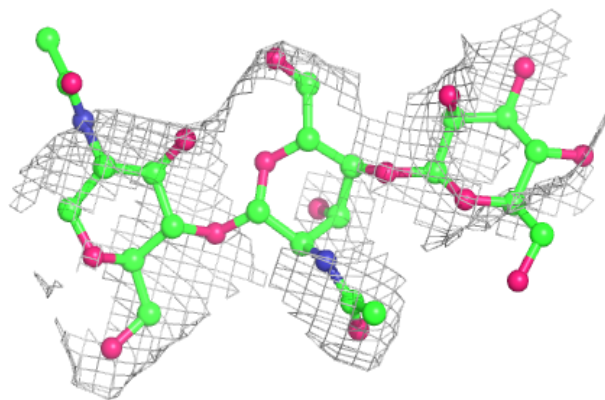


Electron density around Chain D:

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

**Electron density around Chain E:**

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



6.4 Ligands [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
5	NAG	A	808	14/15	0.75	0.33	177,190,199,199	0
5	NAG	B	805	14/15	0.89	0.51	178,196,214,220	0
5	NAG	A	807	14/15	0.90	0.17	143,152,171,171	0
5	NAG	B	804	14/15	0.92	0.27	150,178,187,187	0

6.5 Other polymers [i](#)

There are no such residues in this entry.