



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:31 AM UTC

PDB ID : 5MYB / pdb_00005myb
Title : Homodimerization of Tie2 Fibronectin-like domains 2 and 3 in space group P21
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Deposited on : 2017-01-26
Resolution : 2.60 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

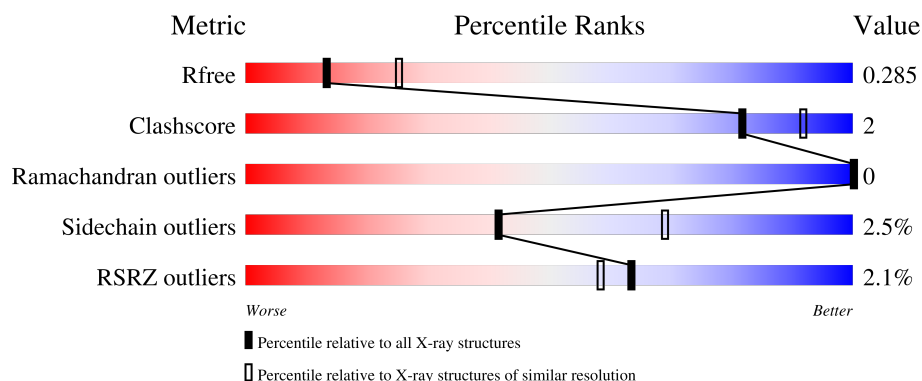
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	54% 43%
1	B	333	55% 43%
2	C	3	33% 67%
3	D	2	100%

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	C	2	-	-	X	-
2	BMA	C	3	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3123 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	190	Total	C	N	O	0	0	0
			1471	934	251	286			
1	B	191	Total	C	N	O	0	0	0
			1467	929	254	284			

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

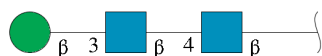
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Chain	Residue	Modelled	Actual	Comment	Reference
A	745	GLY	-	expression tag	UNP Q02763
A	746	ARG	-	expression tag	UNP Q02763
A	747	HIS	-	expression tag	UNP Q02763
A	748	HIS	-	expression tag	UNP Q02763
A	749	HIS	-	expression tag	UNP Q02763
A	750	HIS	-	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

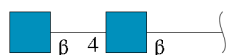
- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



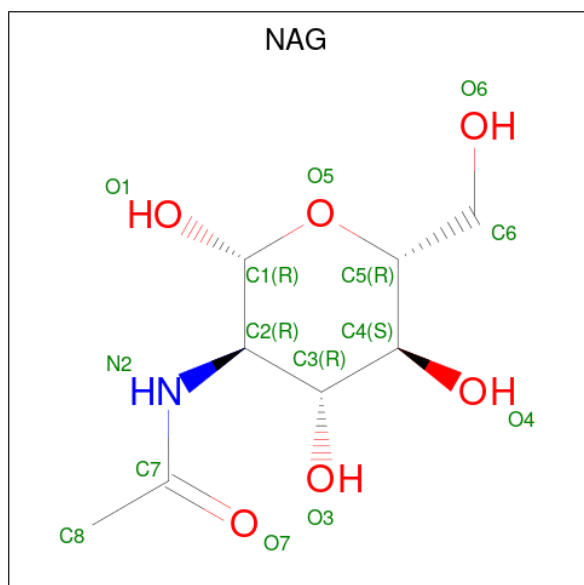
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 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
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	21	Total	O	0	0
			21	21		
5	B	41	Total	O	0	0
			41	41		

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.46Å 48.49Å 80.67Å 90.00° 111.09° 90.00°	Depositor
Resolution (Å)	39.80 – 2.60 39.80 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (39.80-2.60) 99.0 (39.80-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.222 , 0.278 0.231 , 0.285	Depositor DCC
R_{free} test set	1054 reflections (6.00%)	wwPDB-VP
Wilson B-factor (Å ²)	89.9	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 75.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.020 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3123	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% 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: NAG, BMA

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	0.53	0/1505	0.78	2/2066 (0.1%)
1	B	0.51	0/1500	0.74	0/2059
All	All	0.52	0/3005	0.76	2/4125 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	619	THR	CA-C-N	6.67	133.70	121.70
1	A	619	THR	C-N-CA	6.67	133.70	121.70

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	1471	0	1414	3	0
1	B	1467	0	1405	3	0
2	C	39	0	34	9	0
3	D	28	0	25	0	0
4	A	28	0	26	0	0
4	B	28	0	26	0	0
5	A	21	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	41	0	0	3	0
All	All	3123	0	2930	15	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 2.

All (15) 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)
5:A:901:HOH:O	2:C:3:BMA:O3	1.53	1.15
2:C:2:NAG:H62	2:C:3:BMA:H2	1.39	1.01
1:B:695:THR:OG1	5:B:901:HOH:O	1.85	0.94
2:C:2:NAG:H62	2:C:3:BMA:C2	2.07	0.85
2:C:2:NAG:H4	2:C:3:BMA:O2	1.79	0.83
1:B:557:THR:OG1	5:B:902:HOH:O	2.13	0.65
2:C:2:NAG:H62	2:C:3:BMA:C1	2.35	0.56
2:C:2:NAG:H4	2:C:3:BMA:C2	2.37	0.55
2:C:2:NAG:C6	2:C:3:BMA:C1	2.86	0.54
1:A:549:LEU:HB3	1:A:629:LEU:HD11	1.91	0.52
2:C:2:NAG:H4	2:C:3:BMA:HO2	1.77	0.50
1:B:723:PRO:HB3	5:B:904:HOH:O	2.13	0.49
1:A:610:GLN:HB3	1:A:632:TRP:CE2	2.49	0.47
1:A:610:GLN:HB3	1:A:632:TRP:CD2	2.55	0.41
5:A:912:HOH:O	2:C:2:NAG:H83	2.20	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	186/333 (56%)	177 (95%)	9 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	187/333 (56%)	175 (94%)	12 (6%)	0	100	100
All	All	373/666 (56%)	352 (94%)	21 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	163/299 (54%)	159 (98%)	4 (2%)	42	69
1	B	161/299 (54%)	157 (98%)	4 (2%)	42	69
All	All	324/598 (54%)	316 (98%)	8 (2%)	42	69

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	567	PHE
1	A	580	ARG
1	A	651	THR
1	A	732	LEU
1	B	651	THR
1	B	670	ILE
1	B	716	ASN
1	B	731	THR

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

Mol	Chain	Res	Type
1	A	590	ASN
1	A	622	GLN
1	A	641	GLN
1	A	652	HIS
1	B	590	ASN

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Mol	Chain	Res	Type
1	B	698	GLN
1	B	716	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 ⓘ

5 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	0.72	0	17,19,21	1.91	3 (17%)
2	NAG	C	2	2	14,14,15	0.46	0	17,19,21	1.81	3 (17%)
2	BMA	C	3	2	11,11,12	0.33	0	15,15,17	0.98	1 (6%)
3	NAG	D	1	3,1	14,14,15	0.37	0	17,19,21	2.11	3 (17%)
3	NAG	D	2	3	14,14,15	0.43	0	17,19,21	0.98	1 (5%)

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	-	3/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	C	3	2	-	2/2/19/22	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

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	NAG	C1-O5-C5	7.06	121.65	112.19
2	C	1	NAG	C1-O5-C5	6.38	120.74	112.19
2	C	2	NAG	C1-O5-C5	5.94	120.15	112.19
2	C	3	BMA	C1-C2-C3	2.70	113.57	109.64
2	C	2	NAG	C4-C3-C2	2.68	114.95	111.02
2	C	1	NAG	C2-N2-C7	2.64	126.44	122.90
3	D	1	NAG	C2-N2-C7	2.39	126.10	122.90
2	C	2	NAG	C3-C4-C5	2.36	114.50	110.23
3	D	2	NAG	C1-O5-C5	2.35	115.34	112.19
3	D	1	NAG	C1-C2-N2	2.16	113.84	110.43
2	C	1	NAG	C1-C2-N2	2.09	113.72	110.43

There are no chirality outliers.

All (8) torsion outliers are listed below:

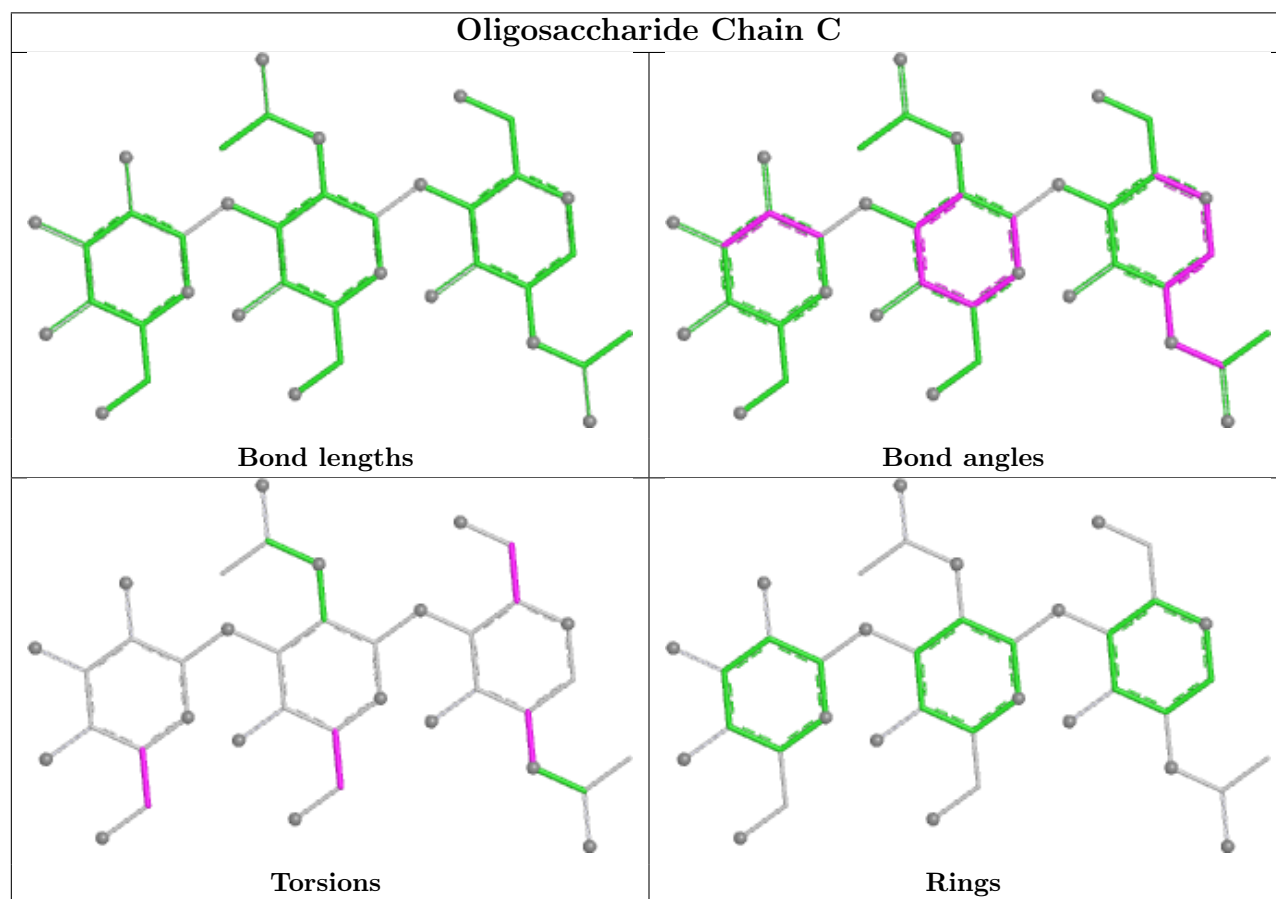
Mol	Chain	Res	Type	Atoms
2	C	3	BMA	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C3-C2-N2-C7
3	D	1	NAG	C3-C2-N2-C7
2	C	1	NAG	C1-C2-N2-C7
2	C	2	NAG	O5-C5-C6-O6

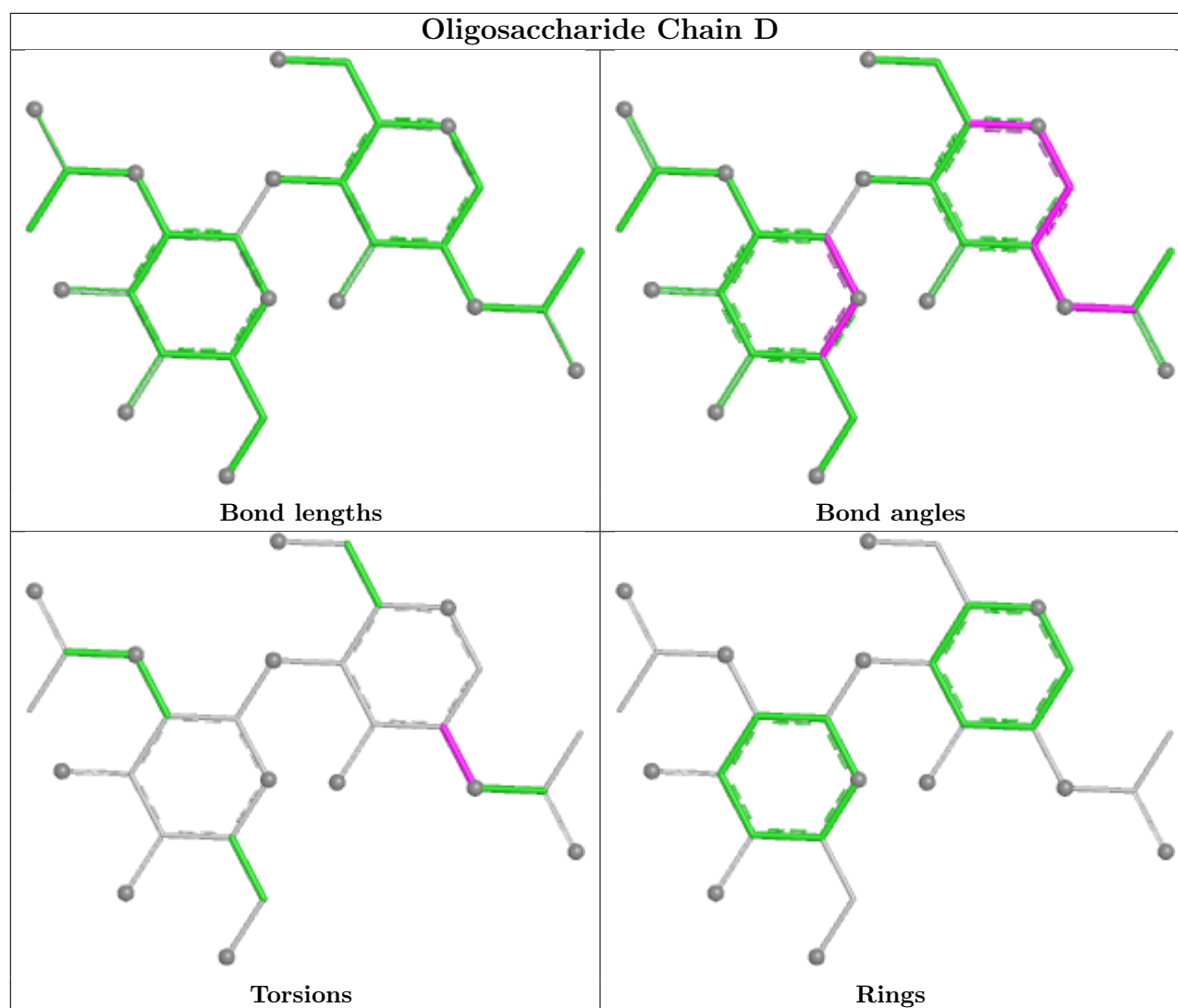
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	BMA	8	0
2	C	2	NAG	8	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](#)

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	$\# Z > 2$
4	NAG	B	801	1	14,14,15	0.30	0	17,19,21	1.37	3 (17%)
4	NAG	B	802	1	14,14,15	0.40	0	17,19,21	0.84	0
4	NAG	A	804	1	14,14,15	0.37	0	17,19,21	1.48	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	805	1	14,14,15	0.55	0	17,19,21	1.19	2 (11%)

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	NAG	B	801	1	-	3/6/23/26	0/1/1/1
4	NAG	B	802	1	-	2/6/23/26	0/1/1/1
4	NAG	A	804	1	-	3/6/23/26	0/1/1/1
4	NAG	A	805	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	801	NAG	C2-N2-C7	2.92	126.82	122.90
4	B	801	NAG	O5-C1-C2	-2.90	106.81	111.29
4	A	805	NAG	C2-N2-C7	2.88	126.77	122.90
4	A	804	NAG	C8-C7-N2	2.82	120.79	116.12
4	A	804	NAG	O5-C1-C2	-2.74	107.05	111.29
4	A	804	NAG	C2-N2-C7	2.58	126.35	122.90
4	B	801	NAG	C8-C7-N2	2.54	120.34	116.12
4	A	805	NAG	C8-C7-N2	2.31	119.95	116.12
4	A	804	NAG	C1-O5-C5	2.07	114.96	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	804	NAG	C8-C7-N2-C2
4	A	804	NAG	O7-C7-N2-C2
4	A	805	NAG	C8-C7-N2-C2
4	A	805	NAG	O7-C7-N2-C2
4	B	801	NAG	C8-C7-N2-C2
4	B	801	NAG	O7-C7-N2-C2
4	B	802	NAG	O5-C5-C6-O6
4	B	802	NAG	C4-C5-C6-O6
4	A	804	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	801	NAG	O5-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	190/333 (57%)	0.05	4 (2%) 63 58	71, 101, 137, 172	0
1	B	191/333 (57%)	0.39	4 (2%) 63 58	73, 117, 160, 191	0
All	All	381/666 (57%)	0.22	8 (2%) 63 58	71, 108, 154, 191	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	724	ALA	3.2
1	A	572	ASP	3.0
1	B	602	LEU	2.9
1	A	724	ALA	2.6
1	B	543	LEU	2.4
1	A	734	GLU	2.3
1	A	571	GLU	2.2
1	B	567	PHE	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 [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.

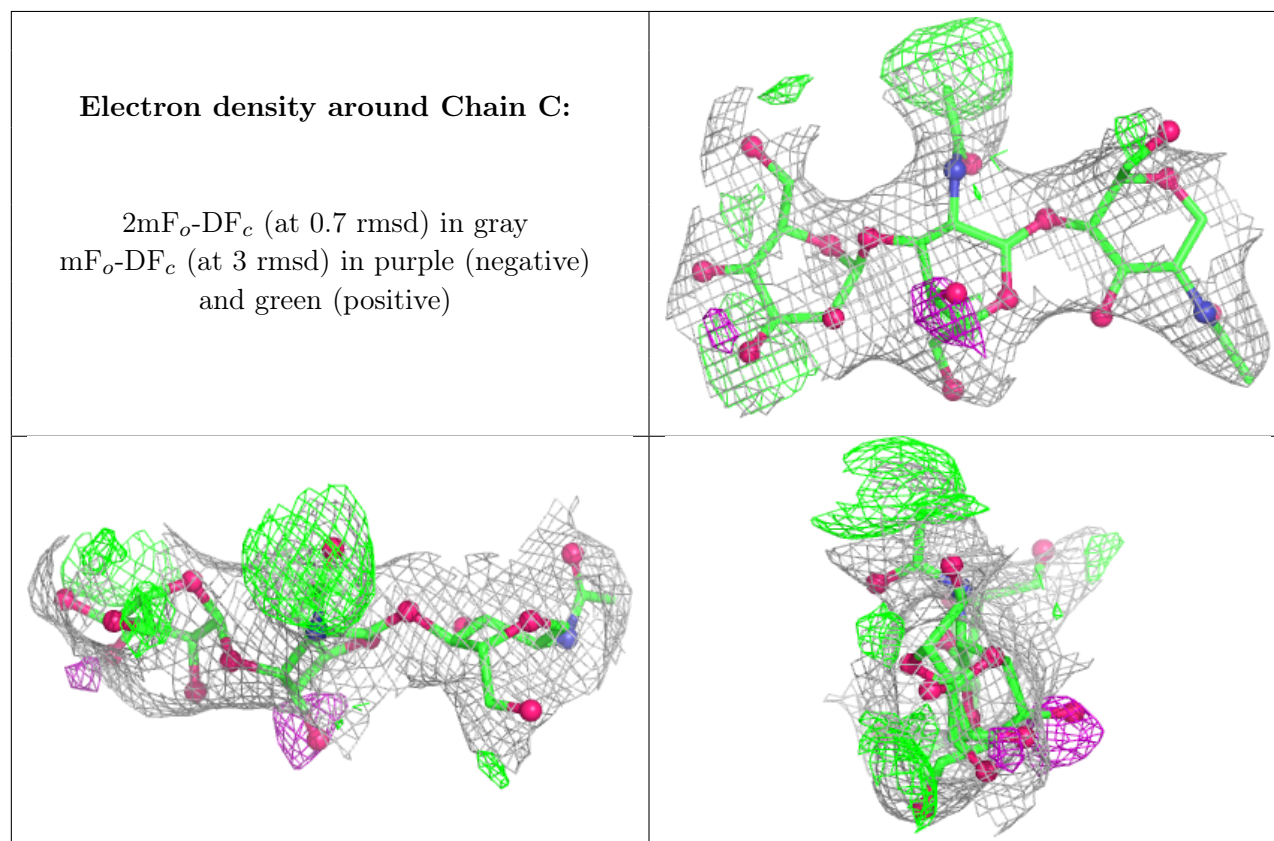
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.34	0.15	117,128,146,149	0

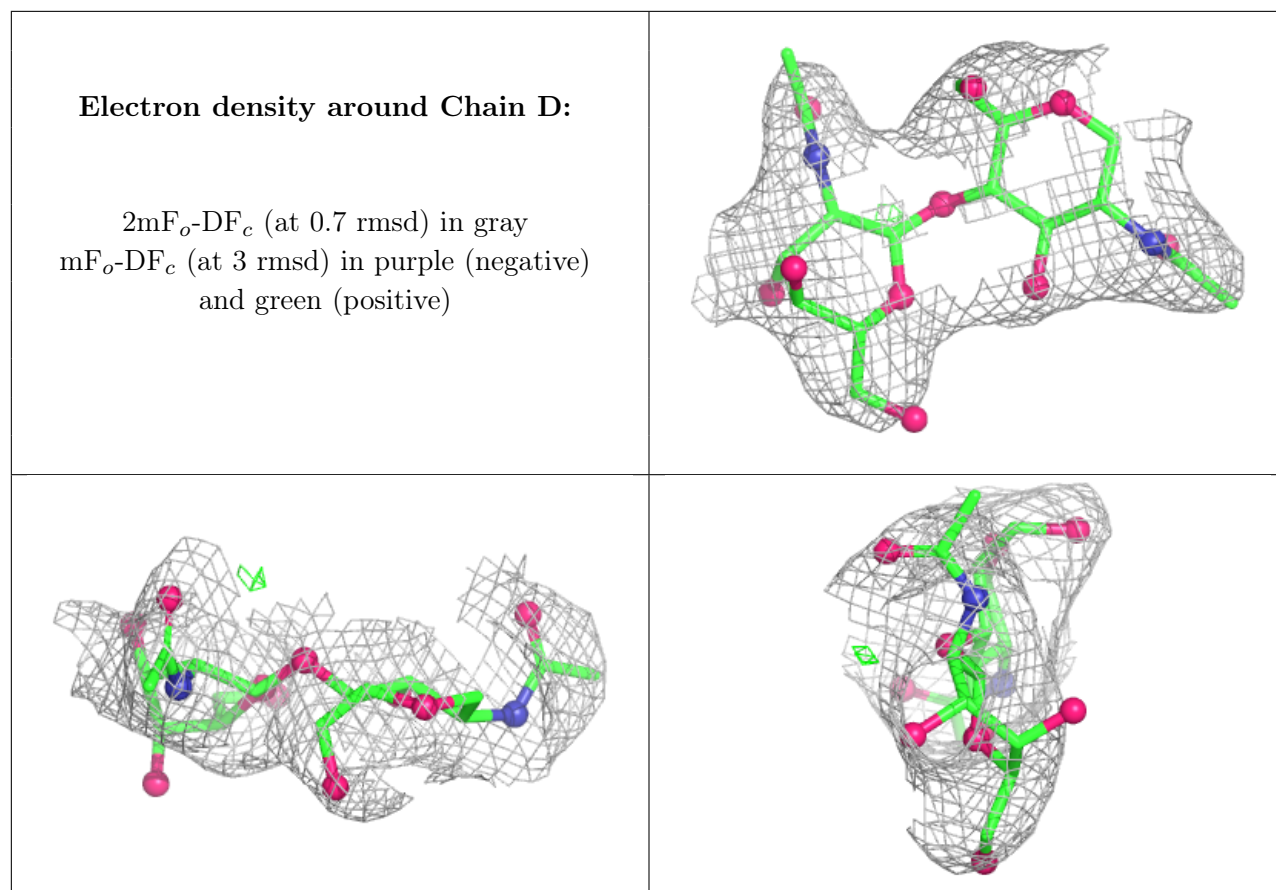
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BMA	C	3	11/12	0.42	0.13	122,137,146,148	0
3	NAG	D	2	14/15	0.73	0.10	134,145,158,159	0
2	NAG	C	1	14/15	0.79	0.12	103,127,135,137	0
3	NAG	D	1	14/15	0.87	0.09	103,121,126,137	0

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($\text{\AA}^2$)	Q<0.9
4	NAG	A	804	14/15	0.29	0.13	122,137,145,155	0
4	NAG	A	805	14/15	0.46	0.11	138,159,172,173	0
4	NAG	B	801	14/15	0.46	0.12	143,162,171,175	0
4	NAG	B	802	14/15	0.70	0.10	135,158,162,163	0

6.5 Other polymers [i](#)

There are no such residues in this entry.