

wwPDB X-ray Structure Validation Summary Report (i)

Jan 7, 2024 – 07:15 pm GMT

PDB ID : 6FKM

Title: Drosophila Plexin A in complex with Semaphorin 1b

Authors: Rozbesky, D.; Harlos, K.; Jones, E.Y.

Deposited on : 2018-01-24

Resolution : 2.96 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

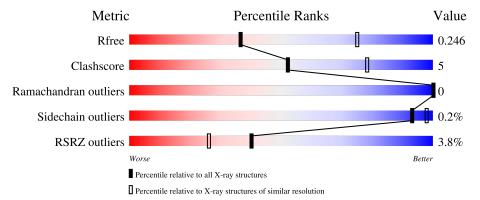
Validation Pipeline (wwPDB-VP) : 2.36

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 2.96 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 <=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 chair	n		
1	A	715	61%	10%	28%	
2	В	578	75%		13%	12%
3	С	5	40%	60%		
3	D	5	60%		40%	

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
3	MAN	D	4	-	-	-	X
4	NAG	A	1003	-	-	=	X



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8119 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 Plexin A, isoform A.

Mol	Chain	Residues		\mathbf{At}	oms			ZeroOcc	AltConf	Trace
1	Λ	512	Total	С	N	О	S	0	0	0
1	A	312	3931	2470	656	779	26	0	U	

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLU	=	expression tag	UNP Q9V491
A	26	THR	-	expression tag	UNP Q9V491
A	27	GLY	-	expression tag	UNP Q9V491
A	731	GLY	-	expression tag	UNP Q9V491
A	732	THR	-	expression tag	UNP Q9V491
A	733	LYS	ı	expression tag	UNP Q9V491
A	734	HIS	-	expression tag	UNP Q9V491
A	735	HIS	-	expression tag	UNP Q9V491
A	736	HIS	-	expression tag	UNP Q9V491
A	737	HIS	-	expression tag	UNP Q9V491
A	738	HIS	-	expression tag	UNP Q9V491
A	739	HIS	-	expression tag	UNP Q9V491

• Molecule 2 is a protein called MIP07328p.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	510	Total 4010	C 2543	N 698	O 750	S 19	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	34	GLU	-	expression tag	UNP Q7KK54
В	35	THR	-	expression tag	UNP Q7KK54
В	36	GLY	-	expression tag	UNP Q7KK54
В	603	GLY	-	expression tag	UNP Q7KK54

Continued on next page...



Continued from previous page...

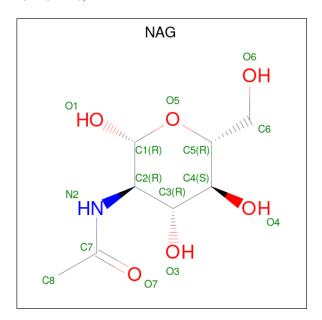
Chain	Residue	Modelled	Actual	Comment	Reference
В	604	THR	-	expression tag	UNP Q7KK54
В	605	LYS	-	expression tag	UNP Q7KK54
В	606	HIS	-	expression tag	UNP Q7KK54
В	607	HIS	-	expression tag	UNP Q7KK54
В	608	HIS	-	expression tag	UNP Q7KK54
В	609	HIS	-	expression tag	UNP Q7KK54
В	610	HIS	_	expression tag	UNP Q7KK54
В	611	HIS	-	expression tag	UNP Q7KK54

• Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	A	ton	ns	ZeroOcc	AltConf	Trace
3	С	5	Total 61			0	0	0
3	D	5	Total 61	C 34		0	0	0

• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





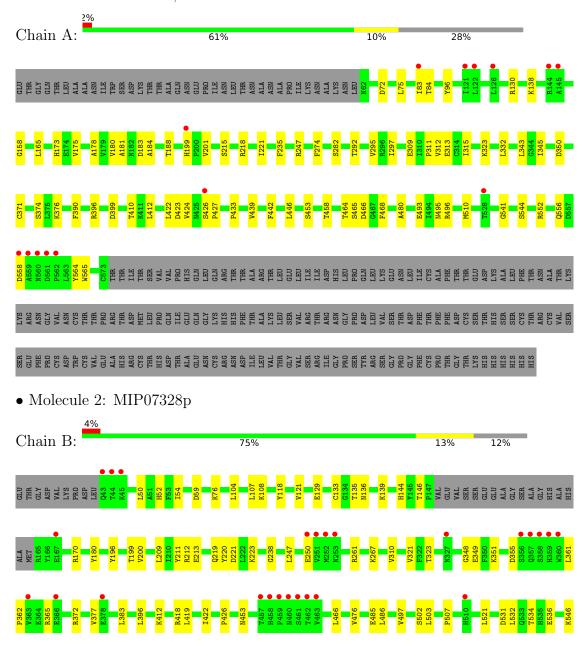
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
1	Λ	1	Total C N O	0	0
4	Λ	1	14 8 1 5	0	0
1	Λ	1	Total C N O	0	0
4	Λ	1	14 8 1 5	0	0
1	Λ	1	Total C N O	0	0
4	Α	1	14 8 1 5	0	0
1	Λ	1	Total C N O	0	0
4	Α	1	14 8 1 5	0	0



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: Plexin A, isoform A





F547 G548	L553 Q554 S555	\$558	A563	T266	H569	ILE	ARG	ASP	ALA	P.P.	1 5	GLU	THE	VAL	SER	PHE	VAL	THR	ME I	PRO	PRO	PRO	THR	GLU	GLO GLN	LYS	LEU	LEU	TYR	SER	WAT	GL.Y	SER	GLY	THR	LYS	HIS	HIS	HIS	HIS	HIS
--------------	----------------------	-------	------	------	------	-----	-----	-----	-----	------	-----	-----	-----	-----	-----	-----	-----	-----	------	-----	-----	-----	-----	-----	------------	-----	-----	-----	-----	-----	-----	------	-----	-----	-----	-----	-----	-----	-----	-----	-----

 $\bullet \ \, Molecule \ 3: \ alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-$

Chain C: 40% 60%

NAG1 NAG2 BMA3 MAN4 MAN5

 $\bullet \ \, Molecule \ 3: \ alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-$

Chain D: 60% 40%

NAG1
NAG2
BMA3
MAN4
MAN5



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	130.94Å 195.09Å 124.84Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.86 - 2.96	Depositor
rtesolution (A)	76.86 - 2.96	EDS
% Data completeness	93.8 (76.86-2.96)	Depositor
(in resolution range)	88.0 (76.86-2.96)	EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.43 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.13rc2_2986: ???)	Depositor
D D.	0.186 , 0.246	Depositor
R, R_{free}	0.186 , 0.246	DCC
R_{free} test set	1515 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	63.5	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31, 38.7	EDS
L-test for twinning ²	$ < L > = 0.47, < L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8119	wwPDB-VP
Average B, all atoms $(Å^2)$	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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, MAN, 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		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.32	0/4010	0.52	0/5450	
2	В	0.30	0/4108	0.51	0/5582	
All	All	0.31	0/8118	0.51	0/11032	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3931	0	3831	49	0
2	В	4010	0	3928	42	0
3	С	61	0	52	0	0
3	D	61	0	52	0	0
4	A	56	0	51	1	0
All	All	8119	0	7914	88	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 5.

The worst 5 of 88 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:311:PRO:HG2	1:A:433:PRO:HB3	1.66	0.77
2:B:348:GLY:O	2:B:372:ARG:NH1	2.17	0.77
2:B:209:LEU:HD13	2:B:211:TYR:HB2	1.76	0.68
1:A:199:HIS:O	1:A:201:VAL:N	2.25	0.66
1:A:464:THR:HG22	1:A:466:ASP:H	1.59	0.65

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	Percer	ntiles
1	A	510/715 (71%)	487 (96%)	23 (4%)	0	100	100
2	В	506/578 (88%)	481 (95%)	25 (5%)	0	100	100
All	All	1016/1293 (79%)	968 (95%)	48 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	A	452/633 (71%)	450 (100%)	2 (0%)	91 96		
2	В	447/502~(89%)	447 (100%)	0	100 100		
All	All	899/1135 (79%)	897 (100%)	2 (0%)	93 98		



All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	ILE
1	A	371	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	GLN

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	Trno	Chain	Dog	Link	Bo	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	С	1	3,2	14,14,15	0.34	0	17,19,21	0.48	0
3	NAG	С	2	3	14,14,15	0.29	0	17,19,21	0.48	0
3	BMA	С	3	3	11,11,12	0.89	0	15,15,17	1.62	2 (13%)
3	MAN	С	4	3	11,11,12	1.01	0	15,15,17	1.04	2 (13%)
3	MAN	С	5	3	11,11,12	0.91	1 (9%)	15,15,17	1.20	2 (13%)
3	NAG	D	1	3,2	14,14,15	0.31	0	17,19,21	0.51	0
3	NAG	D	2	3	14,14,15	0.35	0	17,19,21	0.50	0
3	BMA	D	3	3	11,11,12	0.83	0	15,15,17	0.76	0
3	MAN	D	4	3	11,11,12	0.94	1 (9%)	15,15,17	1.22	2 (13%)



Mol	Type	Chain	Pog	Link	Bo	ond leng	$ ag{ths}$	В	ond ang	les
WIOI	Mol Type Cha	Chain	$\operatorname{ain} \mid \operatorname{Res} \mid$	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	D	5	3	11,11,12	0.82	0	15,15,17	1.09	1 (6%)

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	С	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	С	2	3	-	2/6/23/26	0/1/1/1
3	BMA	С	3	3	-	2/2/19/22	0/1/1/1
3	MAN	С	4	3	-	0/2/19/22	0/1/1/1
3	MAN	С	5	3	-	1/2/19/22	0/1/1/1
3	NAG	D	1	3,2	-	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	-	2/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
3	С	5	MAN	C1-C2	2.52	1.58	1.52
3	D	4	MAN	C1-C2	2.43	1.57	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathrm{Ideal}(^{o})$
3	С	3	BMA	C1-C2-C3	-3.94	104.82	109.67
3	С	3	BMA	O3-C3-C2	3.87	117.41	109.99
3	D	4	MAN	C1-O5-C5	3.42	116.82	112.19
3	D	5	MAN	C1-O5-C5	3.12	116.42	112.19
3	С	5	MAN	C1-O5-C5	2.85	116.05	112.19

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Atoms
3	С	2	NAG	O5-C5-C6-O6
3	С	3	BMA	O5-C5-C6-O6

Continued on next page...



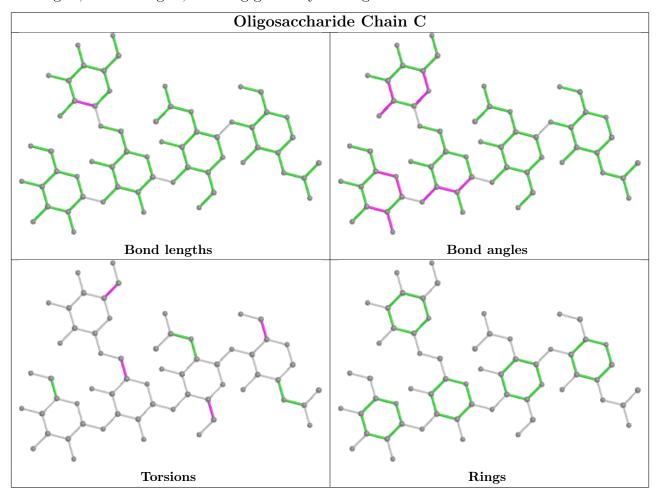
Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	С	2	NAG	C4-C5-C6-O6
3	С	3	BMA	C4-C5-C6-O6
3	С	1	NAG	O5-C5-C6-O6

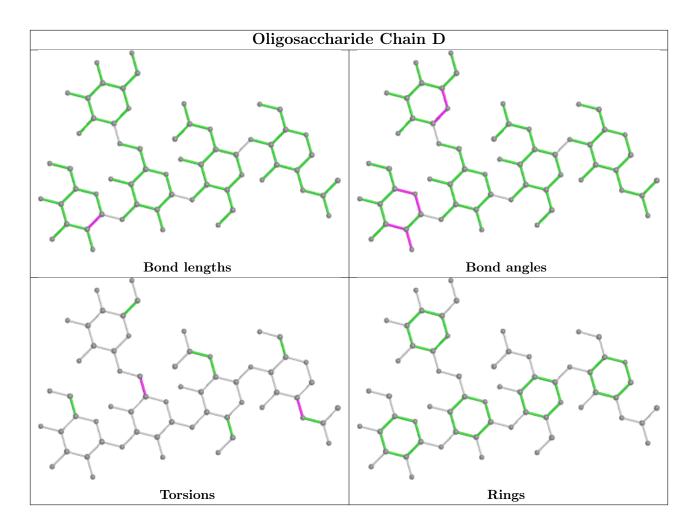
There are no ring outliers.

No monomer is involved in short contacts.

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







5.6 Ligand geometry (i)

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).

Mal	Type	Chain	Res	Link	Bo	Bond lengths			Bond angles		
Mol	Туре		nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
4	NAG	A	1000	1	14,14,15	0.23	0	17,19,21	0.78	0	
4	NAG	A	1003	1	14,14,15	0.60	1 (7%)	17,19,21	0.44	0	
4	NAG	A	1002	1	14,14,15	0.44	0	17,19,21	0.76	0	
4	NAG	A	1001	1	14,14,15	0.22	0	17,19,21	0.58	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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1000	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1003	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1002	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1001	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$Ideal(\AA)$
4	A	1003	NAG	C1-C2	2.04	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	NAG	O5-C5-C6-O6
4	A	1002	NAG	C4-C5-C6-O6
4	A	1003	NAG	C1-C2-N2-C7
4	A	1000	NAG	C3-C2-N2-C7
4	A	1003	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	NAG	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^{th} 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	$\langle { m RSRZ} \rangle$	# RSRZ > 2		$OWAB(Å^2)$	Q<0.9
1	A	512/715 (71%)	0.20	14 (2%) 54	38	39, 62, 125, 188	0
2	В	510/578 (88%)	0.30	25 (4%) 29	18	36, 64, 153, 248	0
All	All	1022/1293 (79%)	0.25	39 (3%) 40	26	36, 63, 139, 248	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	253	ASN	9.3
2	В	356	SER	8.8
2	В	462	THR	7.1
2	В	363	VAL	6.9
2	В	358	SER	6.9

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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	MAN	D	4	11/12	0.59	0.40	124,165,183,187	0
3	MAN	С	5	11/12	0.61	0.26	114,165,172,174	0
3	BMA	D	3	11/12	0.70	0.29	170,177,186,188	0
3	MAN	D	5	11/12	0.72	0.40	141,158,167,168	0
3	BMA	С	3	11/12	0.74	0.19	136,144,162,168	0

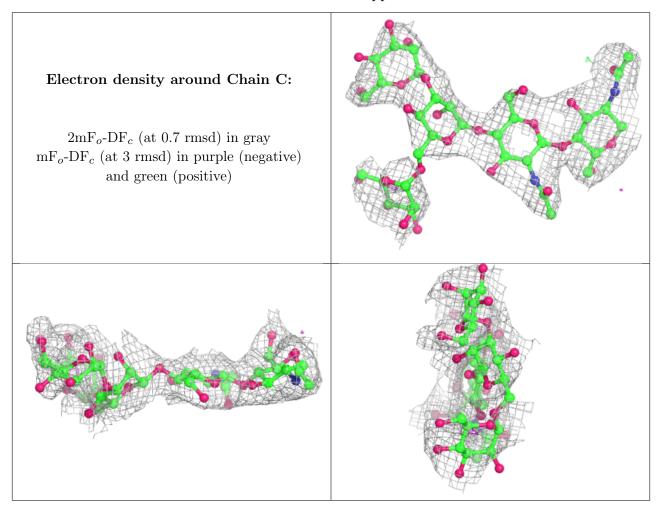
Continued on next page...



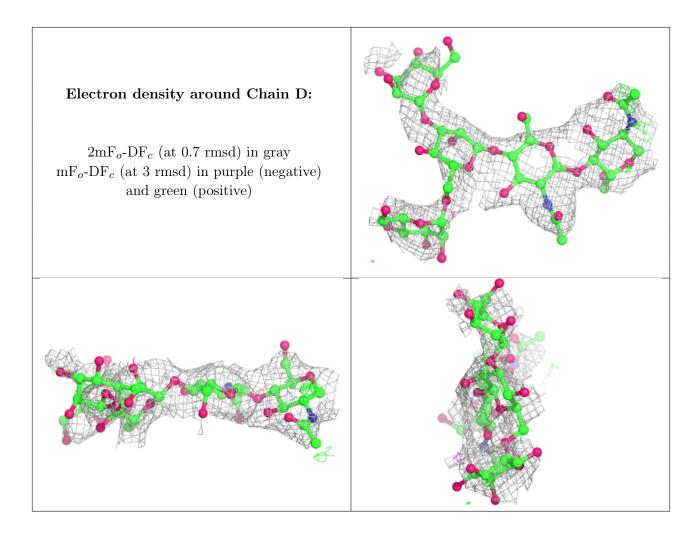
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	MAN	С	4	11/12	0.82	0.19	105,125,136,136	0
3	NAG	D	2	14/15	0.90	0.24	103,136,148,162	0
3	NAG	D	1	14/15	0.91	0.19	97,114,119,128	0
3	NAG	С	2	14/15	0.93	0.19	66,83,105,123	0
3	NAG	С	1	14/15	0.96	0.14	43,54,70,83	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^{th} 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	$ m B ext{-}factors(\AA^2)$	Q<0.9
4	NAG	A	1002	14/15	0.67	0.29	102,140,163,169	0
4	NAG	A	1001	14/15	0.80	0.28	96,121,126,128	0
4	NAG	A	1003	14/15	0.80	0.41	139,149,156,156	0
4	NAG	A	1000	14/15	0.92	0.21	88,101,114,124	0

6.5 Other polymers (i)

There are no such residues in this entry.

