

Full wwPDB X-ray Structure Validation Report (i)

Oct 6, 2021 – 07:17 am BST

PDB ID : 7ALT

Title : Structure of Drosophila Serrate C2-DSL-EGF1-EGF2

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Deposited on : 2020-10-07

Resolution : 2.03 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.23.2

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

Refmac: 5.8.0267

CCP4 : 7.1.010 (Gargrove) roteins) : Engh & Huber (2001)

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

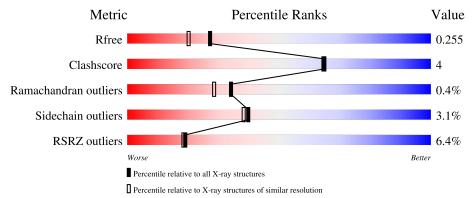
Validation Pipeline (wwPDB-VP) : 2.23.2

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 2.03 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{A})}) \end{array}$
R_{free}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 chain						
1	А	270	88%	10%					
1	71	210	6%	10%	•				
1	В	270	90%	8%	• •				
0	C	9							
2	$^{\circ}$	2	100%						



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8161 atoms, of which 3906 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 Protein serrate.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total 4004	C 1280	H 1944	N 357	O 396	S 27	0	0	0
1	В	265	Total 3930	C 1256	H 1911	N 350	O 386	S 27	0	0	0

• 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	С	9	Total	С	Н	N	О	0	0	0
		2	53	16	25	2	10	U		

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

\mathbf{Mol}	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	В	1	Total Ca 1 1	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		
4	D	1	Total	С	Н	N	О	0	0	
4	D	1	27	8	13	1	5	0	0	
4	D	1	Total	С	Н	N	О	0	0	
4	D		27	8	13	1	5	0		

• Molecule 5 is water.

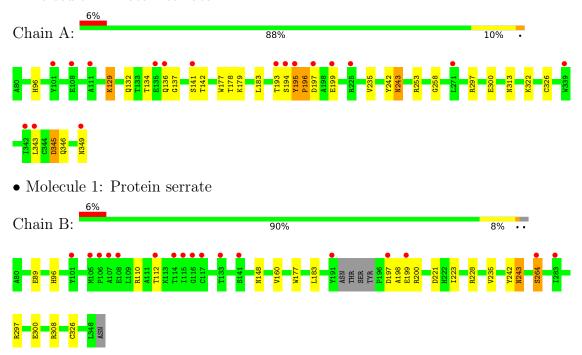
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	58	Total O 58 58	0	0
5	В	60	Total O 60 60	0	0



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: Protein serrate



 $\bullet \ \, \text{Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2$

Chain C: 100%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	70.33Å 49.40Å 93.12Å	Depositor
a, b, c, α , β , γ	90.00° 110.25° 90.00°	Depositor
Resolution (Å)	45.61 - 2.03	Depositor
Resolution (A)	45.61 - 2.03	EDS
% Data completeness	98.9 (45.61-2.03)	Depositor
(in resolution range)	98.9 (45.61-2.03)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.27 (at 2.03Å)	Xtriage
Refinement program	PHENIX dev_3965, PHENIX dev_3965	Depositor
D.D.	0.220 , 0.258	Depositor
R, R_{free}	0.219 , 0.255	DCC
R_{free} test set	1996 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8161	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 39.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2484e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Clasia		nd lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.30	0/2108	0.57	0/2862	
1	В	0.37	$2/2065 \ (0.1\%)$	0.62	1/2800 (0.0%)	
All	All	0.34	$2/4173 \ (0.0\%)$	0.59	1/5662 (0.0%)	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(A)
1	В	264	SER	CB-OG	7.53	1.52	1.42
1	В	264	SER	CA-CB	5.85	1.61	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathbf{Ideal}(^o)$
1	В	264	SER	N-CA-CB	8.86	123.79	110.50

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	2060	1944	1943	20	0
1	В	2019	1911	1909	13	0
2	С	28	25	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	В	1	0	0	0	0
4	В	28	26	26	0	0
5	A	58	0	0	1	0
5	В	60	0	0	1	2
All	All	4255	3906	3903	33	2

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 4.

All (33) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	overlap (Å)
1:A:297:ARG:NH1	1:A:300:GLU:OE1	2.04	0.90
1:B:197:ASP:O	1:B:200:ARG:HG2	1.84	0.77
1:B:221:ASP:OD2	1:B:228:ARG:NH2	2.20	0.75
1:A:195:TYR:HB3	1:A:196:PRO:CD	2.28	0.63
1:B:297:ARG:NH2	1:B:300:GLU:OE1	2.35	0.57
1:A:195:TYR:HB3	1:A:196:PRO:HD3	1.86	0.57
1:B:197:ASP:OD1	1:B:198:ALA:N	2.38	0.57
1:B:197:ASP:H	1:B:200:ARG:HH11	1.58	0.51
1:A:142:THR:O	1:A:142:THR:CG2	2.60	0.49
1:A:132:GLN:OE1	1:A:137:GLY:HA3	2.13	0.49
1:A:177:TRP:CZ2	1:A:235:VAL:HG21	2.48	0.48
1:A:134:THR:HG23	1:A:136:GLN:HG2	1.95	0.48
1:B:177:TRP:CZ2	1:B:235:VAL:HG21	2.48	0.48
1:A:197:ASP:OD2	1:A:199:GLU:CG	2.60	0.48
1:A:343:LEU:HB2	1:A:345:ASP:OD1	2.13	0.48
1:A:129:LYS:HE2	1:A:137:GLY:O	2.15	0.47
1:A:345:ASP:OD2	1:A:346:GLN:NE2	2.48	0.47
1:A:322:LYS:HG3	1:A:345:ASP:HB3	1.97	0.46
1:B:197:ASP:OD2	1:B:199:GLU:OE1	2.33	0.46
1:A:197:ASP:OD2	1:A:199:GLU:OE2	2.34	0.45
1:A:242:TYR:O	1:A:243:ASN:CB	2.65	0.45
1:B:183:LEU:HD12	1:B:183:LEU:C	2.36	0.45
1:B:308:ARG:NE	5:B:512:HOH:O	2.50	0.45
1:A:142:THR:O	1:A:142:THR:HG22	2.17	0.44
1:A:183:LEU:HD12	1:A:183:LEU:C	2.39	0.43
1:B:89:GLU:OE1	1:B:160:VAL:HG22	2.19	0.42
1:B:110:ARG:HG2	1:B:112:THR:HG23	2.02	0.42
1:A:253:ARG:HG2	1:A:258:GLY:O	2.20	0.41

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Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:B:223:ILE:O	1:B:223:ILE:HG22	2.21	0.41
1:A:313:ASN:OD1	5:A:501:HOH:O	2.22	0.41
1:A:178:THR:O	1:A:179:LYS:HB2	2.21	0.41
1:A:132:GLN:OE1	1:A:137:GLY:CA	2.69	0.41
1:B:242:TYR:O	1:B:243:ASN:CB	2.69	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
5:B:501:HOH:O	5:B:505:HOH:O[1_445]	1.76	0.44
5:B:533:HOH:O	5:B:543:HOH:O[2_746]	2.13	0.07

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	Perce	ntiles	
1	A	268/270 (99%)	251 (94%)	15 (6%)	2 (1%)	22	15
1	В	$261/270 \ (97\%)$	246 (94%)	15 (6%)	0	100	100
All	All	529/540 (98%)	497 (94%)	30 (6%)	2 (0%)	34	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	TYR
1	A	196	PRO

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	227/227 (100%)	218 (96%)	9 (4%)	31 28		
1	В	222/227~(98%)	217 (98%)	5 (2%)	50 51		
All	All	449/454 (99%)	435 (97%)	14 (3%)	40 38		

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

Mol	Chain	Res	Type
1	A	96	HIS
1	A	129	LYS
1	A	141	SER
1	A	193	THR
1	A	194	SER
1	A	243	ASN
1	A	326	CYS
1	A	345	ASP
1	A	349	ASN
1	В	96	HIS
1	В	148	ASN
1	В	243	ASN
1	В	264	SER
1	В	326	CYS

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	256	GLN
1	В	256	GLN
1	В	346	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)

2 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	Trme	Type Chain Res I		Link	Bo	ond leng	ths	В	ond ang	gles
	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	С	1	2,1	14,14,15	0.47	0	17,19,21	1.11	2 (11%)
2	NAG	С	2	2	14,14,15	1.12	2 (14%)	17,19,21	1.24	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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	С	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	С	2	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$[Ideal(\AA)]$
2	С	2	NAG	O5-C1	3.54	1.49	1.43
2	С	2	NAG	C1-C2	2.15	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	С	2	NAG	C1-O5-C5	4.79	118.68	112.19
2	С	1	NAG	O5-C1-C2	-2.24	107.75	111.29
2	С	1	NAG	C3-C4-C5	2.05	113.90	110.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

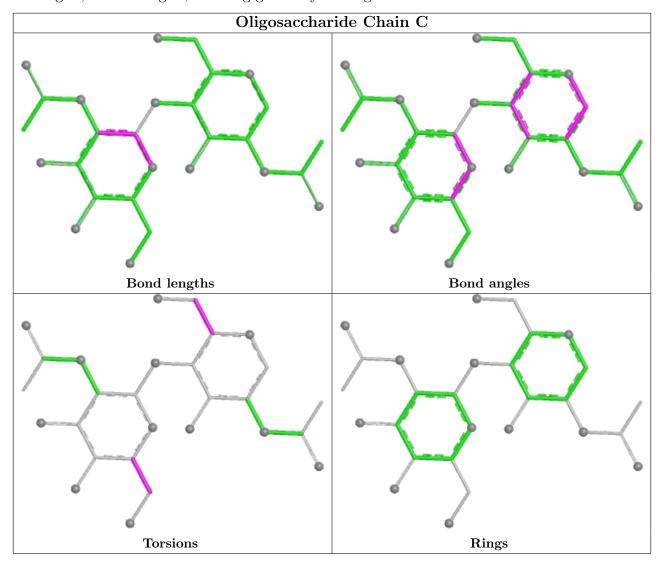


Mol	Chain	Res	Type	Atoms
2	С	1	NAG	C4-C5-C6-O6
2	С	1	NAG	O5-C5-C6-O6
2	С	2	NAG	C4-C5-C6-O6
2	С	2	NAG	O5-C5-C6-O6

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)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	Chain	Chain	Chain	Chain	Chain	Chain	Res	Link	Во	ond leng	ths	В	ond ang	les
	туре		nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2					
4	NAG	В	401	1	14,14,15	0.78	1 (7%)	17,19,21	1.15	2 (11%)					
4	NAG	В	402	1	14,14,15	1.21	1 (7%)	17,19,21	0.86	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
4	NAG	В	401	1	-	2/6/23/26	0/1/1/1
4	NAG	В	402	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
4	В	402	NAG	O5-C1	3.91	1.50	1.43
4	В	401	NAG	O5-C1	-2.09	1.40	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^o)$
4	В	401	NAG	C1-O5-C5	3.19	116.51	112.19
4	В	401	NAG	C3-C4-C5	2.80	115.23	110.24
4	В	402	NAG	O5-C1-C2	-2.31	107.64	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	401	NAG	C1-C2-N2-C7
4	В	402	NAG	C4-C5-C6-O6
4	В	402	NAG	O5-C5-C6-O6
4	В	401	NAG	C3-C2-N2-C7



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^{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	$\langle { m RSRZ} \rangle$	$\# \mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	A	270/270 (100%)	0.61	17 (6%) 20 19	23, 35, 77, 113	0
1	В	265/270~(98%)	0.62	17 (6%) 19 18	25, 39, 61, 103	0
All	All	535/540 (99%)	0.61	34 (6%) 19 18	23, 37, 67, 113	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	115	ILE	7.6
1	В	108	GLU	5.5
1	A	194	SER	4.4
1	A	108	GLU	4.4
1	В	106	PRO	4.1
1	A	136	GLN	3.9
1	A	141	SER	3.6
1	A	195	TYR	3.5
1	В	107	ALA	3.5
1	A	349	ASN	3.5
1	В	114	THR	3.1
1	A	193	THR	3.0
1	A	342	ILE	3.0
1	A	135	GLU	2.9
1	В	264	SER	2.9
1	В	105	MET	2.9
1	В	101	TYR	2.8
1	A	199	GLU	2.8
1	A	343	LEU	2.7
1	В	141	SER	2.7
1	В	197	ASP	2.6
1	A	101	TYR	2.6
1	A	271	LEU	2.4
1	В	116	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	В	112	THR	2.3
1	В	191	TYR	2.2
1	A	197	ASP	2.2
1	В	117	CYS	2.2
1	A	111	ALA	2.2
1	В	199	GLU	2.1
1	В	133	THR	2.1
1	В	283	ILE	2.1
1	A	339	TRP	2.0
1	A	225	ARG	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.

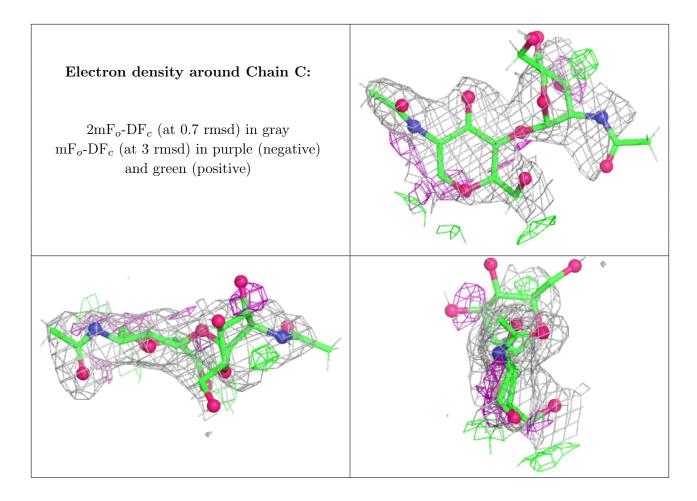
6.3 Carbohydrates (i)

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, 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
2	NAG	С	2	14/15	0.69	0.38	70,89,113,113	0
2	NAG	С	1	14/15	0.83	0.20	40,58,73,76	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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	NAG	В	402	14/15	0.72	0.20	46,64,83,87	0
4	NAG	В	401	14/15	0.76	0.26	66,81,98,103	0
3	CA	В	403	1/1	0.87	0.13	54,54,54,54	0
3	CA	A	401	1/1	0.95	0.14	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.

