

wwPDB X-ray Structure Validation Summary Report (i)

Nov 6, 2023 – 12:18 AM EST

PDB ID	:	148L
Title	:	A COVALENT ENZYME-SUBSTRATE INTERMEDIATE WITH SACCHA-
		RIDE DISTORTION IN A MUTANT T4 LYSOZYME
Authors	:	Kuroki, R.; Weaver, L.H.; Matthews, B.W.
Deposited on		
Resolution	:	1.90 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:

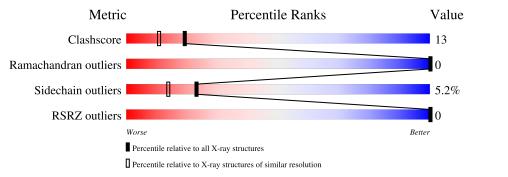
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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 chai	n	
1	Е	164	67%	27% •	
2	S	4	50%	50%	
3	А	2	100%		



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 1525 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 T4 LYSOZYME.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Е	163	Total 1317	C 827	N 244	0 241	${ m S}{ m 5}$	0	2	1

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	26	GLU	THR	conflict	UNP P00720
Е	54	THR	CYS	conflict	UNP P00720
E	97	ALA	CYS	conflict	UNP P00720

• Molecule 2 is a protein called SUBSTRATE CLEAVED FROM CELL WALL OF ESCHERICHIA COLI.

Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf	Trace
2	\mathbf{S}	4	Total 32	C 18	N 5	O 9	0	0	0

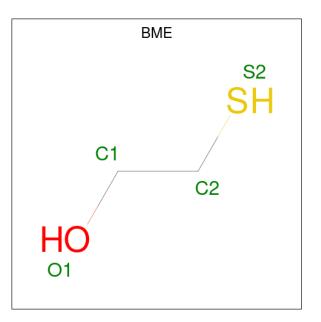
• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid.



Mol	Chain	Residues	I	Aton	ns		ZeroOcc	AltConf	Trace
3	А	2	Total 32	C 19	N 2	O 11	0	0	0

• Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).





Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
4	Е	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	0 1	S 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Е	127	Total O 127 127	0	0
5	S	13	Total O 13 13	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.

Chain E:	67%	27%	
M E E B B B B B B B B B B B B B B B B B	22 724 127 129 129 129 129 128 128 128 128 128 128 128 128 128 128	150 R52 D61 D61 D61 D61 D63 R68 R68 R68 R68 R78 R78 R78 R78 R78 R78 R78 R78 R78 R7	R80 D92 E108 T109 M119 M120
Q123 Q124 R126 D127 D127 D127 P143 N144 A146 A146 X146 X146	F153 F153 M158 M159 F162 M163 LEU		
• Molecule 2: SUBST	TRATE CLEAVED F	ROM CELL WALL OF	ESCHERICHIA COLI
Chain S:	50%	50%	

• Molecule 1: T4 LYSOZYME

A166 E167 K169 A170

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid

Chain A:

100%

MUB1 NAG2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	50.90Å 67.30 Å 49.60 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 - 1.90	Depositor
Resolution (A)	18.59 - 1.76	EDS
% Data completeness	(Not available) $(20.00-1.90)$	Depositor
(in resolution range)	78.7 (18.59-1.76)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.15 (at 1.77 \text{\AA})$	Xtriage
Refinement program	TNT	Depositor
D D.	0.168 , (Not available)	Depositor
R, R_{free}	0.159 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	11.1	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.29,84.6	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.033 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1525	wwPDB-VP
Average B, all atoms $(Å^2)$	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.50% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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: BME, DAL, API, NAG, FGA, MUB

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		Bo	nd lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	Е	1.00	7/1337~(0.5%)	1.71	30/1799~(1.7%)	
2	S	1.07	0/4	1.47	0/4	
All	All	1.00	7/1341~(0.5%)	1.71	30/1803~(1.7%)	

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Ε	128	GLU	CD-OE2	6.79	1.33	1.25
1	Е	62	GLU	CD-OE2	6.72	1.33	1.25
1	Е	64	GLU	CD-OE1	6.29	1.32	1.25
1	Е	108	GLU	CD-OE2	6.27	1.32	1.25
1	Е	11	GLU	CD-OE1	6.22	1.32	1.25

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	Е	76	ARG	NE-CZ-NH1	14.88	127.74	120.30
1	Е	76	ARG	NE-CZ-NH2	-11.21	114.69	120.30
1	Е	125	ARG	NE-CZ-NH1	9.51	125.05	120.30
1	Е	80	ARG	NE-CZ-NH2	9.18	124.89	120.30
1	Е	47	ASP	CB-CG-OD2	-8.54	110.62	118.30

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ε	1317	0	1342	35	0
2	S	32	0	20	1	0
3	А	32	0	27	0	0
4	Е	4	0	6	0	1
5	Ε	127	0	0	8	0
5	S	13	0	0	1	0
All	All	1525	0	1395	36	1

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.

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 13.

The worst 5 of 36 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:E:1:MET:HG2	1:E:158:TRP:CD2	2.19	0.77
1:E:145[B]:ARG:HB3	5:E:441:HOH:O	1.84	0.75
1:E:144:ASN:H	1:E:145[B]:ARG:HH21	1.33	0.75
1:E:8[B]:ARG:O	1:E:8[B]:ARG:HD2	1.95	0.66
1:E:146:ALA:O	1:E:150:ILE:HG13	1.95	0.66

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
4:E:174:BME:S2	4:E:174:BME:S2[2_565]	2.04	0.16

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	Ε	163/164~(99%)	162 (99%)	1 (1%)	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 side chain 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	Ε	137/137~(100%)	129~(94%)	8 (6%)	20 10		

5 of 8 residues with a non-rotameric side chain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	Ε	162	LYS
1	Е	145[B]	ARG
1	Е	119	ARG
1	Е	76	ARG
1	Ε	145[A]	ARG

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

Mol	Chain	Res	Type
1	Ε	140	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	Mol Type Chain Res		Chain Res Link		Bo	Bond lengths			Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
2	API	S	169	2	$10,\!11,\!12$	2.11	3 (30%)	$11,\!13,\!15$	1.47	2 (18%)	
2	FGA	S	167	2	7,8,9	0.83	0	7,9,11	1.13	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	API	S	169	2	-	2/12/12/14	-
2	FGA	S	167	2	-	1/7/8/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	169	API	OXT-C	-5.24	1.20	1.42
2	S	169	API	O3-C7	2.85	1.30	1.22
2	S	169	API	O4-C7	-2.59	1.22	1.30

All (2) bond angle outliers are listed below:

M	bl	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2		S	169	API	O4-C7-C6	3.05	123.77	113.38
2		S	169	API	OXT-C-CA	2.37	120.87	111.52

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	S	169	API	OXT-C-CA-C3
2	S	169	API	OXT-C-CA-N
2	S	167	FGA	OXT-C-CA-N

There are no ring outliers.

No monomer is involved in short contacts.



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	Turne	Chain	Res	Link	Bo	ond leng	$_{\rm ths}$	Bond angles		
10101	Type	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	MUB	А	1	3,1,2	17,18,20	1.08	1 (5%)	21,24,28	<mark>5.58</mark>	13 (61%)
3	NAG	А	2	3	14,14,15	0.77	0	17,19,21	1.50	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MUB	А	1	3,1,2	-	2/10/29/34	0/1/1/1
3	NAG	А	2	3	-	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(Å)
3	А	1	MUB	O7-C7	2.11	1.28	1.23

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	А	1	MUB	C3-C2-N2	17.43	142.87	110.58
3	А	1	MUB	O5-C1-C2	10.08	127.20	111.29
3	А	1	MUB	O3-C3-C2	-7.96	90.17	108.85
3	А	1	MUB	O6-C6-C5	-5.87	91.15	111.29
3	А	1	MUB	O4-C4-C3	-5.34	95.79	109.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

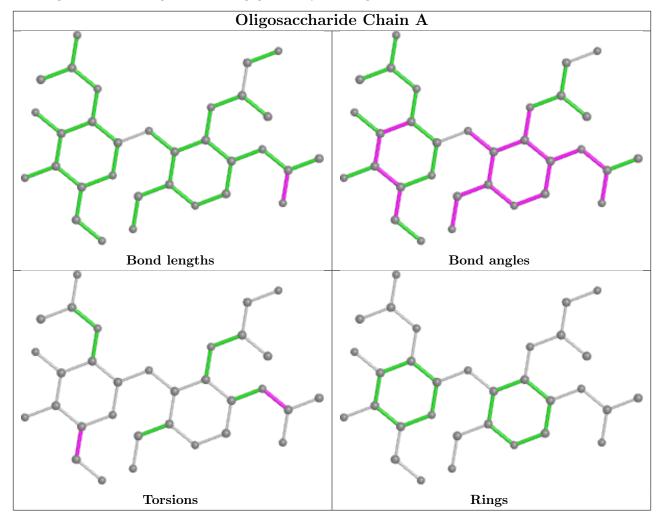


Mol	Chain	Res	Type	Atoms
3	А	1	MUB	O7-C7-N2-C2
3	А	1	MUB	C8-C7-N2-C2
3	А	2	NAG	C4-C5-C6-O6
3	А	2	NAG	O5-C5-C6-O6

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)

1 ligand is 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



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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		
	WIOI	Type	Ullaili	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
	4	BME	Е	174	-	3, 3, 3	0.60	0	$1,\!2,\!2$	0.00	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
4	BME	Ε	174	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Е	174	BME	O1-C1-C2-S2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	174	BME	0	1

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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	Ε	163/164~(99%)	-0.72	0 100 100	3, 13, 31, 47	0
2	S	1/4~(25%)	-1.10	0 100 100	8, 8, 8, 8	0
All	All	164/168~(97%)	-0.73	0 100 100	3, 13, 31, 47	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains (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	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q < 0.9
2	API	S	169	12/13	0.97	0.07	$5,\!8,\!12,\!13$	0
2	FGA	S	167	9/10	0.97	0.06	3,6,12,13	0
2	DAL	S	170	6/6	0.97	0.08	8,24,30,32	0

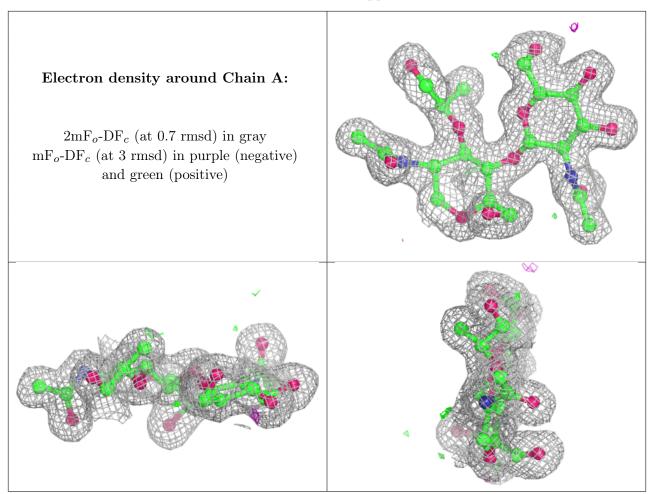
6.3 Carbohydrates (i)

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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	MUB	А	1	18/20	0.98	0.05	$3,\!7,\!12,\!13$	0
3	NAG	А	2	14/15	0.98	0.05	6,9,16,20	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-





charide. 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
4	BME	Ε	174	4/4	0.80	0.14	$26,\!36,\!53,\!68$	0

6.5 Other polymers (i)

There are no such residues in this entry.

