



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7Q4T / pdb_00007q4t
Title : Structure of the Pseudomonas aeruginosa bacteriophage JG004 endolysin Pae87 bound to a peptidoglycan fragment.
Authors : Seoane-Blanco, M.; van Raaij, M.J.
Deposited on : 2021-11-02
Resolution : 1.27 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

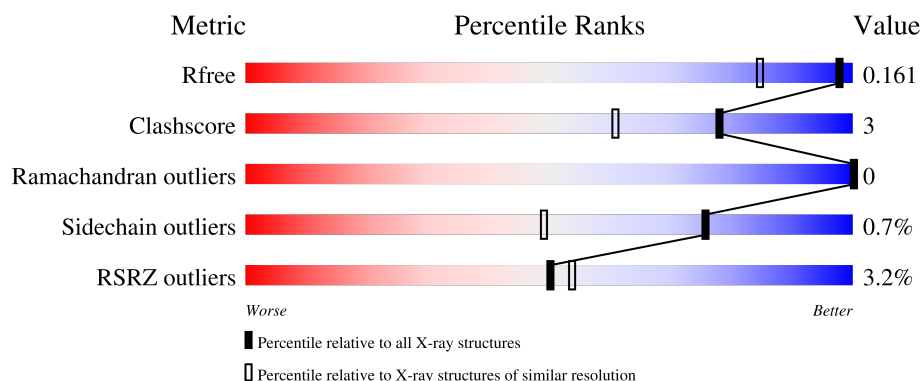
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.27 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	2836 (1.30-1.26)
Clashscore	190562	2911 (1.30-1.26)
Ramachandran outliers	187476	2841 (1.30-1.26)
Sidechain outliers	187428	2840 (1.30-1.26)
RSRZ outliers	180081	2832 (1.30-1.26)

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	AAA	206	
2	LbL	2	
3	LLL	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 1743 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 Endolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	187	Total	C	N	O	S	0	5	0
			1506	966	262	272	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-19	MET	-	initiating methionine	UNP F4YDQ3
AAA	-18	GLY	-	expression tag	UNP F4YDQ3
AAA	-17	SER	-	expression tag	UNP F4YDQ3
AAA	-16	SER	-	expression tag	UNP F4YDQ3
AAA	-15	HIS	-	expression tag	UNP F4YDQ3
AAA	-14	HIS	-	expression tag	UNP F4YDQ3
AAA	-13	HIS	-	expression tag	UNP F4YDQ3
AAA	-12	HIS	-	expression tag	UNP F4YDQ3
AAA	-11	HIS	-	expression tag	UNP F4YDQ3
AAA	-10	HIS	-	expression tag	UNP F4YDQ3
AAA	-9	SER	-	expression tag	UNP F4YDQ3
AAA	-8	SER	-	expression tag	UNP F4YDQ3
AAA	-7	GLY	-	expression tag	UNP F4YDQ3
AAA	-6	LEU	-	expression tag	UNP F4YDQ3
AAA	-5	VAL	-	expression tag	UNP F4YDQ3
AAA	-4	PRO	-	expression tag	UNP F4YDQ3
AAA	-3	ARG	-	expression tag	UNP F4YDQ3
AAA	-2	GLY	-	expression tag	UNP F4YDQ3
AAA	-1	SER	-	expression tag	UNP F4YDQ3
AAA	0	HIS	-	expression tag	UNP F4YDQ3

- Molecule 2 is a protein called ALA-DGL.

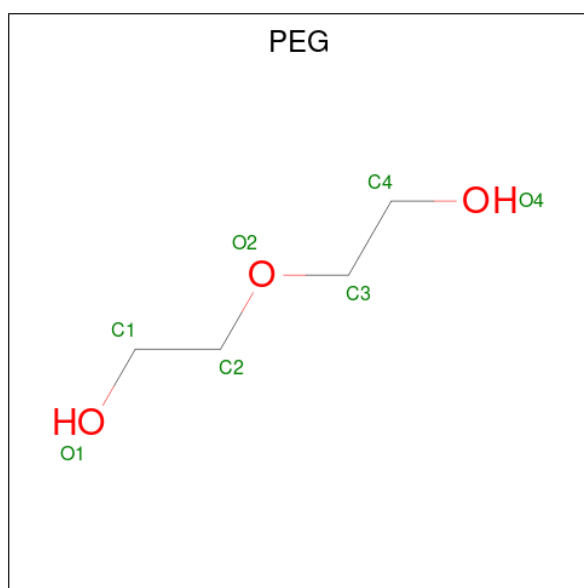
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	LbL	2	Total	C	N	O	0	0	0
			15	8	2	5			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	LLL	2	Total	C	N	O	0	1	0
			35	20	2	13			

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			7	4	3		
4	AAA	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	LbL	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	110	Total 114	O 114	0	4
6	LbL	7	Total 7	O 7	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: Endolysin

Chain AAA: 



- Molecule 2: ALA-DGL

Chain LbL: 



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

Chain LLL: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.58Å 61.17Å 69.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.85 – 1.27 45.84 – 1.27	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.85-1.27) 99.8 (45.84-1.27)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 1.27Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.130 , 0.161 0.130 , 0.161	Depositor DCC
R_{free} test set	2454 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.826	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	1743	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.40% 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: PEG, NAG, MUB, DGL, EDO

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	AAA	0.88	0/1562	1.02	0/2100
2	LbL	0.38	0/4	0.74	0/4
All	All	0.88	0/1566	1.02	0/2104

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	AAA	1506	0	1490	7	0
2	LbL	15	0	9	0	0
3	LLL	35	0	21	0	0
4	AAA	14	0	20	3	0
5	AAA	48	0	72	3	0
5	LbL	4	0	6	0	0
6	AAA	114	0	0	2	0
6	LbL	7	0	0	0	0
All	All	1743	0	1618	9	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 3.

All (9) 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:AAA:136:ASN:HD22	4:AAA:202:PEG:H32	1.44	0.81
1:AAA:136:ASN:HD22	4:AAA:202:PEG:C3	2.19	0.50
5:AAA:205:EDO:H12	6:AAA:373:HOH:O	2.16	0.46
1:AAA:43:ILE:HA	1:AAA:101:SER:O	2.16	0.45
1:AAA:112:TRP:CD1	1:AAA:120[A]:VAL:HG22	2.51	0.45
1:AAA:136:ASN:ND2	4:AAA:202:PEG:H32	2.24	0.43
1:AAA:115:LEU:O	1:AAA:140:ARG:HD3	2.19	0.43
1:AAA:143:LYS:HG2	5:AAA:203:EDO:H22	2.01	0.42
5:AAA:205:EDO:C1	6:AAA:373:HOH:O	2.69	0.41

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	AAA	190/206 (92%)	186 (98%)	4 (2%)	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	AAA	157/168 (94%)	156 (99%)	1 (1%)	78	53

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	0	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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 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	DGL	LbL	4	2	8,9,9	1.07	1 (12%)	8,11,11	0.97	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	DGL	LbL	4	2	-	1/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	LbL	4	DGL	OXT-C	-2.20	1.23	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	LbL	4	DGL	OE2-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

3 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$
3	MUB	LLL	1[A]	-	18,19,20	0.36	0	21,26,28	0.69	0
3	MUB	LLL	1[B]	-	18,19,20	0.34	0	21,26,28	0.68	0
3	NAG	LLL	2	3	14,14,15	0.83	1 (7%)	17,19,21	0.71	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
3	MUB	LLL	1[A]	-	-	1/11/32/34	0/1/1/1
3	MUB	LLL	1[B]	-	-	1/11/32/34	0/1/1/1
3	NAG	LLL	2	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	LLL	2	NAG	O4-C4	2.02	1.48	1.43

There are no bond angle outliers.

There are no chirality outliers.

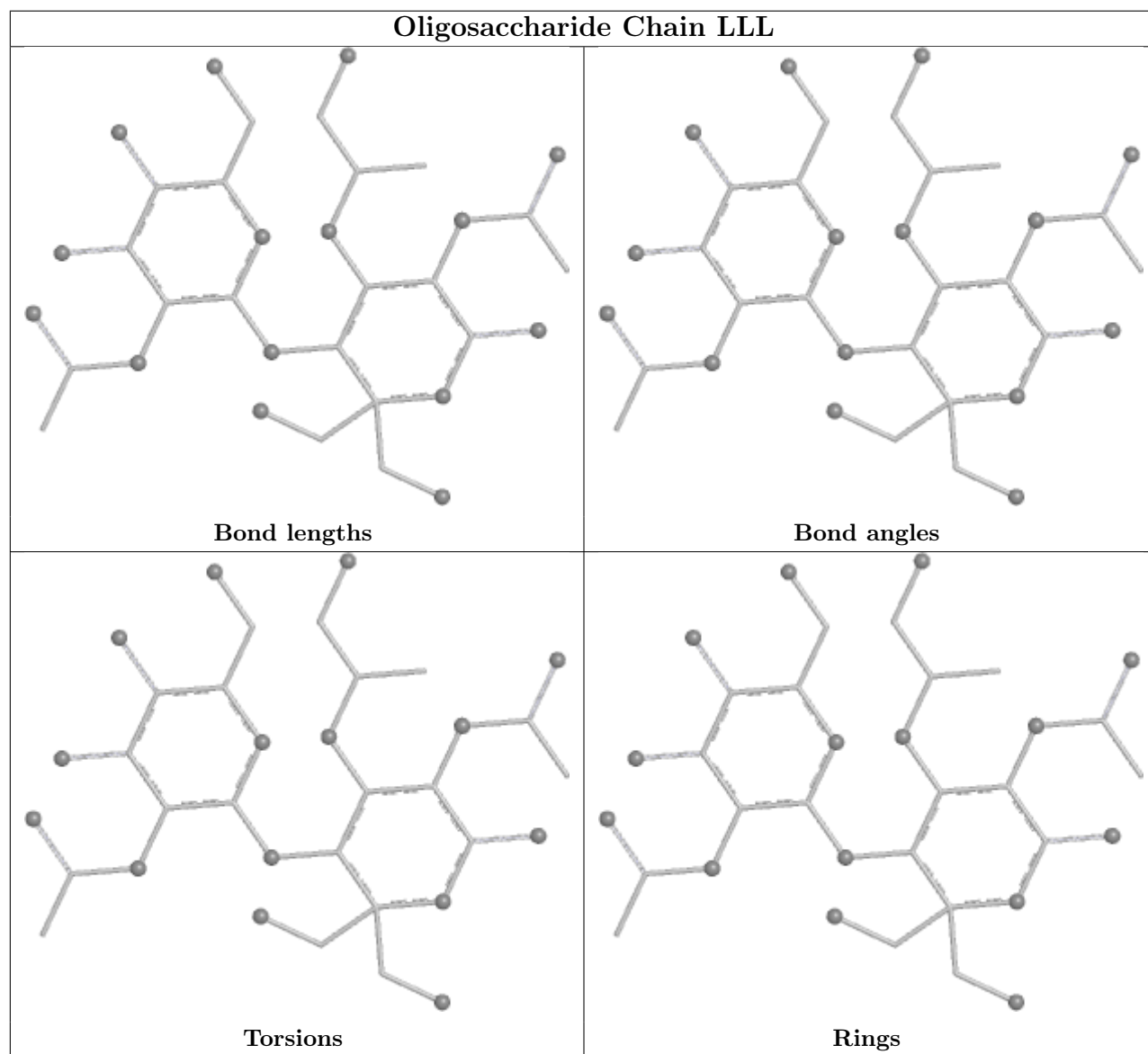
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	LLL	1[A]	MUB	O10-C10-C9-C11
3	LLL	1[B]	MUB	O10-C10-C9-C11

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](#)

15 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	EDO	AAA	208	-	3,3,3	0.11	0	2,2,2	0.10	0
4	PEG	AAA	202	-	6,6,6	0.21	0	5,5,5	0.10	0
5	EDO	AAA	205	-	3,3,3	0.11	0	2,2,2	0.15	0
5	EDO	AAA	209	-	3,3,3	0.05	0	2,2,2	0.09	0
5	EDO	AAA	203	-	3,3,3	0.53	0	2,2,2	1.05	0
5	EDO	AAA	212	-	3,3,3	0.07	0	2,2,2	0.06	0
5	EDO	AAA	204	-	3,3,3	0.28	0	2,2,2	0.43	0
5	EDO	AAA	210	-	3,3,3	0.09	0	2,2,2	0.11	0
4	PEG	AAA	201	-	6,6,6	0.18	0	5,5,5	0.09	0
5	EDO	AAA	214	-	3,3,3	0.13	0	2,2,2	0.17	0
5	EDO	LbL	101	-	3,3,3	0.03	0	2,2,2	0.08	0
5	EDO	AAA	213	-	3,3,3	0.09	0	2,2,2	0.12	0
5	EDO	AAA	207	-	3,3,3	0.13	0	2,2,2	0.14	0
5	EDO	AAA	206	-	3,3,3	0.03	0	2,2,2	0.02	0
5	EDO	AAA	211	-	3,3,3	0.06	0	2,2,2	0.03	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
5	EDO	AAA	208	-	-	1/1/1/1	-
4	PEG	AAA	202	-	-	2/4/4/4	-
5	EDO	AAA	205	-	-	0/1/1/1	-
5	EDO	AAA	209	-	-	0/1/1/1	-
5	EDO	AAA	203	-	-	0/1/1/1	-
5	EDO	AAA	212	-	-	0/1/1/1	-
5	EDO	AAA	204	-	-	1/1/1/1	-
5	EDO	AAA	210	-	-	1/1/1/1	-
4	PEG	AAA	201	-	-	2/4/4/4	-
5	EDO	AAA	214	-	-	1/1/1/1	-
5	EDO	LbL	101	-	-	1/1/1/1	-
5	EDO	AAA	213	-	-	1/1/1/1	-
5	EDO	AAA	207	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	AAA	206	-	-	1/1/1/1	-
5	EDO	AAA	211	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	201	PEG	O2-C3-C4-O4
4	AAA	202	PEG	O2-C3-C4-O4
5	AAA	210	EDO	O1-C1-C2-O2
5	AAA	204	EDO	O1-C1-C2-O2
5	AAA	206	EDO	O1-C1-C2-O2
5	AAA	208	EDO	O1-C1-C2-O2
4	AAA	201	PEG	C4-C3-O2-C2
4	AAA	202	PEG	O1-C1-C2-O2
5	AAA	213	EDO	O1-C1-C2-O2
5	AAA	214	EDO	O1-C1-C2-O2
5	LbL	101	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	202	PEG	3	0
5	AAA	205	EDO	2	0
5	AAA	203	EDO	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

6.1 Protein, DNA and RNA chains

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	AAA	187/206 (90%)	-0.05	6 (3%) 50 54	10, 18, 36, 61	5 (2%)
2	LbL	1/2 (50%)	0.18	0 100 100	17, 17, 17, 17	0
All	All	188/208 (90%)	-0.05	6 (3%) 50 54	10, 18, 36, 61	5 (2%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	2	ALA	4.3
1	AAA	1	MET	3.4
1	AAA	0	HIS	3.2
1	AAA	60	HIS	3.0
1	AAA	59	GLY	2.8
1	AAA	32	GLY	2.4

6.2 Non-standard residues in protein, DNA, RNA chains

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.

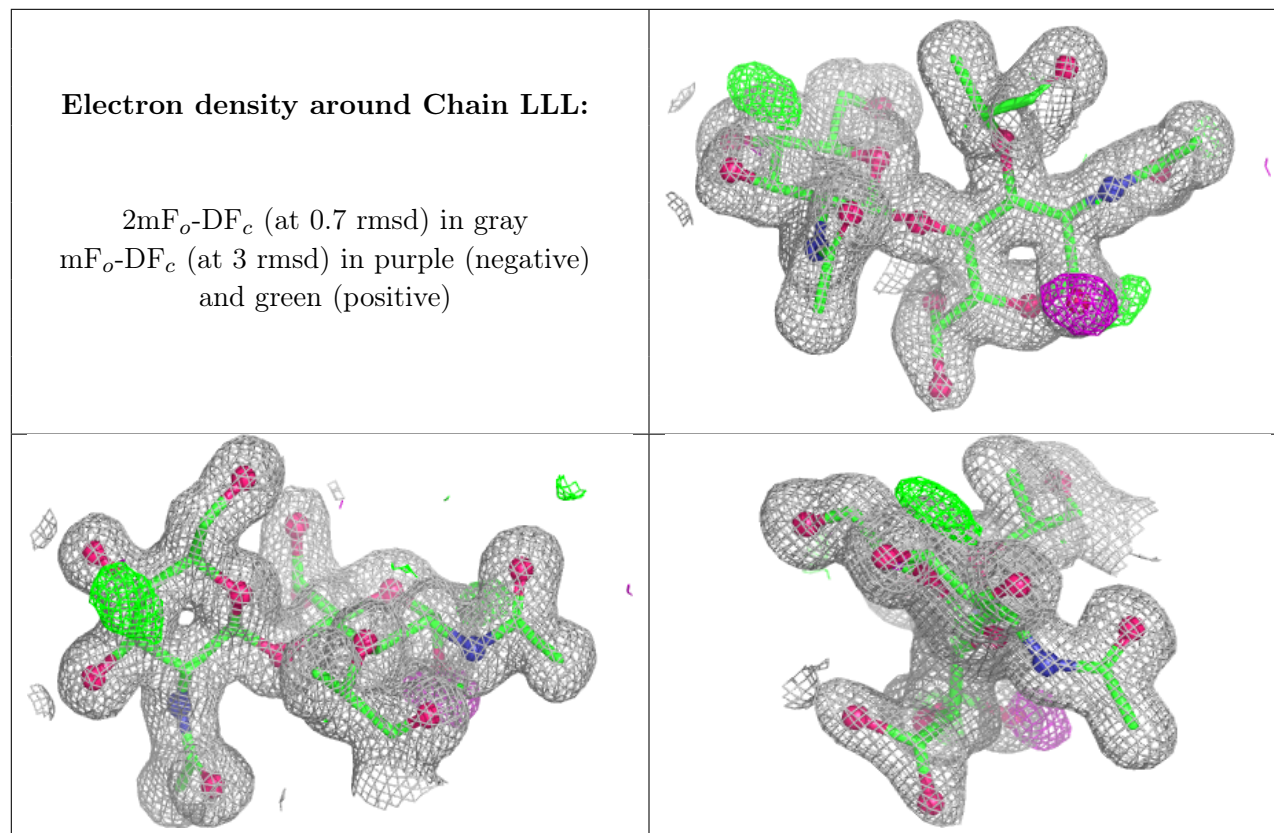
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DGL	LbL	4	10/10	0.96	0.08	19,28,49,57	0

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($\text{\AA}^2$)	Q<0.9
3	MUB	LLL	1[A]	19/20	-	-	15,16,18,23	2
3	MUB	LLL	1[B]	19/20	-	-	15,16,23,24	2
3	NAG	LLL	2	14/15	-	-	14,17,21,21	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 ⓘ

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
5	EDO	AAA	212	4/4	0.64	0.17	33,34,38,40	0
4	PEG	AAA	202	7/7	0.83	0.14	32,38,43,43	0
5	EDO	AAA	210	4/4	0.83	0.15	51,55,56,64	0
5	EDO	AAA	211	4/4	0.83	0.14	39,42,48,49	0
4	PEG	AAA	201	7/7	0.83	0.14	36,44,49,50	0
5	EDO	AAA	214	4/4	0.83	0.13	50,52,57,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	AAA	209	4/4	0.85	0.16	45,50,50,50	0
5	EDO	AAA	205	4/4	0.86	0.14	35,38,39,40	0
5	EDO	AAA	206	4/4	0.88	0.12	34,43,50,53	0
5	EDO	AAA	213	4/4	0.88	0.13	55,58,58,60	0
5	EDO	AAA	204	4/4	0.88	0.12	20,28,38,44	0
5	EDO	LbL	101	4/4	0.88	0.14	44,54,56,57	0
5	EDO	AAA	208	4/4	0.90	0.10	40,43,43,45	0
5	EDO	AAA	207	4/4	0.91	0.12	31,38,41,56	0
5	EDO	AAA	203	4/4	0.95	0.16	14,17,19,30	4

6.5 Other polymers [i](#)

There are no such residues in this entry.